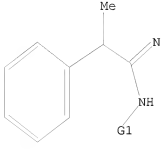
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Me,Et,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 09:08:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 380 TO ITERATE

100.0% PROCESSED 380 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 6431 TO 8769
PROJECTED ANSWERS: 9 TO 360

L2 9 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 09:08:19 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 7373 TO ITERATE

100.0% PROCESSED 7373 ITERATIONS 143 ANSWERS
SEARCH TIME: 00.00.01

L3 143 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 186.10

FILE 'CAPLUS' ENTERED AT 09:08:23 ON 09 JAN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 9 Jan 2009 VOL 150 ISS 3
FILE LAST UPDATED: 8 Jan 2009 (20090108/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l3
L4 62 L3

=> d ibib abs hitstr tot

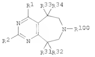
L4 ANSWER 1 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1185770 CAPLUS
DOCUMENT NUMBER: 149:425966
TITLE: Preparation of pyrimido[4,5-d]azepine derivatives as 5-HT2C agonists
INVENTOR(S): Andrews, Mark David; Blagg, Julian; Brennan, Paul Edward; Fish, Paul Vincent; Roberts, Lee Richard; Storer, Robert Ian; Whitlock, Gavin Alistair
PATENT ASSIGNEE(S): Pfizer Limited, UK
SOURCE: PCT Int. Appl., 180pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008117169	A1	20081002	WO 2008-IB731	20080314

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2007-896527P P 20070323

OTHER SOURCE(S): MARPAT 149:425966
GI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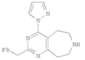
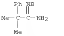
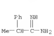

II

AB The title compds. I [R1 = H, alkyl, fluoroalkyl, cycloalkyl, etc.; R2 = (CH2)pPh, CHR6Ph, NR7R8, etc.; R31, R32, R33, R34 = H, alkyl, fluoroalkyl; R6 = alkyl, fluoroalkyl, OH or F; R7 = alkyl, fluoroalkyl, cycloalkyl or fluorocycloalkyl; R8 = alkyl, fluoroalkyl, cycloalkyl, cycloalkylmethyl or fluorocycloalkyl; or NR7R8 = 4-6 membered heterocyclyl optionally

L4 ANSWER 1 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
comprising 1 further heteroatom selected from O and S (said ring being optionally fused to a Ph ring); p = 1-2; R100 = H or NH prodrug moiety] which act as 5-HT2C agonists, were prepd. E.g., a multi-step synthesis of II, starting from 1-tert-Bu 4-Et 5-oxoazepane-1,4-dicarboxylate and 2-phenylacetamidine, was given. II showed Ki of 72.0 nM when tested for 5-HT2C agonistic activity. Pharmaceutical compn. comprising the compd. I is disclosed.
IT 883031-17-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimido[4,5-d]azepines as 5HT2C agonists useful in treatment of diseases)
RN 883031-17-2 CAPLUS
CN Benzeneethanimidamide, α,α-dimethyl- (CA INDEX NAME)



IT 761353-05-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimido[4,5-d]azepines as 5HT2C agonists useful in treatment of diseases)
RN 761353-05-3 CAPLUS
CN Benzeneethanimidamide, α-methyl- (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

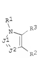
L4 ANSWER 2 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:736475 CAPLUS
DOCUMENT NUMBER: 149:79594
TITLE: Pyrazole derivatives as LXR and FXR modulators and their preparation, pharmaceutical compositions and use in the treatment of diseases
INVENTOR(S): Boren, Brant Clayton; Busch, Brett B.; Gu, Xiao-Hui; Jammalamadaka, Vasu; Lu, Shao-Po; Martin, Richard; Mohan, Raju; Schweiger, Edwin; Stevens, William C., Jr.; Wang, Tie-Lin; Xie, Yinong; Xu, Wei
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 355pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008073825	A1	20080619	WO 2007-US86787	20071207

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2006-869198P P 20061208

OTHER SOURCE(S): MARPAT 149:79594
GI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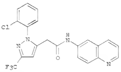
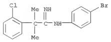

II

AB Compds. of the invention are disclosed, such as compds. of formula I, and pharmaceutically acceptable salts, isomers, or prodrugs thereof, which are useful as modulators of the activity of liver X receptors (LXR) and Farnesoid X receptors (FXR). Pharmaceutical compns. containing the compds.

L4 ANSWER 2 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
and methods of using the compds. are also disclosed. Compds. of formula I wherein J1 is N and J2 is CR4; J1 is CR5 and J2 is N; R1, R3 and R5 are independently (un)substituted biaryl, (un)substituted heterobiaryl, (un)substituted aryl-heteroaryl, (un)substituted (hetero)aryl, etc.; R2 and R4 are independently alkyl, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted alkoxyalkyl, (un)substituted C3-6 cycloalkyl, (un)substituted heteroaryl, etc.; and their pharmaceutically acceptable salts thereof, are claimed. Example compd. II was prepd. by cyanation of 5-(bromomethyl)-1-(2-chlorophenyl)-3-trifluoromethyl-1H-pyrazole; the resulting (1-(-2-chlorophenyl)-3-trifluoromethyl-1H-pyrazol-5-yl)acetonitrile underwent hydrolysis to give (1-(-2-chlorophenyl)-3-trifluoromethyl-1H-pyrazol-5-yl)acetic acid, which underwent amidation with quinolin-6-ylamine to give compd. II. All the invention compds. were evaluated for their LXR and FXR modulatory activity. Form the assay, it was detd. that compd. II exhibited EC50 value < 1 μM.
IT 1033586-82-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of pyrazole derivs. as LXR and FXR modulators useful in the treatment of diseases)
RN 1033586-82-1 CAPLUS
CN Benzeneethanimidamide, N-(4-bromophenyl)-2-chloro-α,α-dimethyl- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:1303013 CAPLUS
DOCUMENT NUMBER: 147:541746
TITLE: Preparation of quinolinones and analogs as antiviral agents
INVENTOR(S): Kumar, Dange V.; Rai, Roopa; Young, Wendy B.; Hu, Huiyong; Riggs, Jennifer R.; Ton, Tony Loc; Green, Michael J.; Hart, Barry P.; Brameld, Kenneth A.; Dener, Jeff M.
PATENT ASSIGNEE(S): Virobay, Inc., USA
SOURCE: PCT Int. Appl., 201pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007130499	A2	20071115	WO 2007-US10702	20070430
WO 2007130499	A3	20080110		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070287699	A1	20071213	US 2007-742461	20070430
PRIORITY APPLN. INFO.:			US 2006-796943P	P 20060501

OTHER SOURCE(S): MARPAT 147:541746
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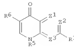
L4 ANSWER 3 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)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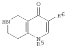
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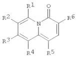
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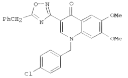
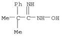
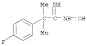

IV

AB Title compds. represented by the formula I & II & III [wherein Z1 = N or CR1; Z2 = N or CR2; Z3 = N or CR4; R1 = H, halo, alkyl, etc.; R2 = H, halo, alkoxy, etc.; R3 = halo, alkyl, aryl, etc.; R4 = H, halo, haloalkyl, etc.; R5 = alkyl, cycloalkylamino, arylamino, etc.; R6 = (un)substituted 1,2,4-oxadiazol-3-yl, 1,2,4-oxadiazol-5-yl, 1,3,4-oxadiazol-2-yl or oxazol-2-yl; and pharmaceutically acceptable salts thereof] were prepared as antiviral agents. For example, IV was provided in a multi-step synthesis starting from reaction of Et 2-cyano-3-ethoxyacrylate with 3,4-dimethoxyphenylamine. The invention compds. showed activity in HCV replicon assays and their formulations were also presented. Thus, the title compds. and their pharmaceutical compns. are useful for the treatment of viral infections, particularly HCV.
IT 957140-71-5, N-Hydroxy-2-methyl-2-phenylpropanimidamide
957140-73-7, 2-(4-Fluorophenyl)-N-hydroxy-2-methylpropanimidamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 4-quinolinones and analogs as antiviral agents)
RN 957140-71-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α,α-dimethyl- (CA INDEX NAME)

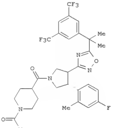


RN 957140-73-7 CAPLUS

L4 ANSWER 3 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
CN Benzeneethanimidamide, 4-fluoro-N-hydroxy-α,α-dimethyl- (CA INDEX NAME)



L4 ANSWER 4 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:1050755 CAPLUS
DOCUMENT NUMBER: 148:385
TITLE: Pyrrolidine-carboxamides and oxadiazoles as potent hNK1 antagonists
AUTHOR(S): Young, Jonathan R.; Eid, Ronsar; Turner, Cherilyn; DeVita, Robert J.; Kurtz, Marc M.; Tsao, Kwei-Lan C.; Chicchi, Gary G.; Wheeldon, Alan; Carlson, Emma; Mills, Sander G.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065-0900, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(19), 5310-5315
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:385
GI


I

AB The preparation and structure-activity relationships of novel pyrrolidine-carboxamides and oxadiazoles are described. Compds. in this series were found to be potent hNK1 antagonists in vitro and efficacious in vivo with minimal interactions with P450 liver enzymes. Oxadiazole analog (I) was determined to have excellent hNK1 binding affinity, functional activity, and a good PD response in vivo.
IT 957476-30-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(pyrrolidine-carboxamides and oxadiazoles as potent hNK1 antagonists)
RN 957476-30-1 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α,α-dimethyl-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

L4 ANSWER 4 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:744613 CAPLUS
DOCUMENT NUMBER: 146:454167
TITLE: 6-alkylthio-4-(1-(2,6-difluorophenyl)alkyl)-1H-[1,3,5]triazin-2-ones (DATs): novel regulators of cell differentiation and proliferation
AUTHOR(S): Ebardelis, Gianlena; Bartolini, Sara; Castellano, Sabrina; Artico, Marino; Fermeno, Nicola; Rotili, Dante; Spadafora, Corrado; Ma, Antonello
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita degli Studi di Salerno, Fisciano, 84084, Italy
SOURCE: ChemMedChem (2006), 1(10), 1073-1080
CODEN: CHEMKG; ISSN: 1860-7179
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:454167
GI

I

AB Novel triazine analogs of 5-alkyl-2-alkylthio-6-(1-(2,6-difluorophenyl)alkyl)-3,4-dihydropyrimidin-4(3H)-ones (F-DABOs), previously described by us as nonnucleoside HIV-1 reverse transcriptase inhibitors (NNRTIs), were tested for their antiproliferative and cytodifferentiating activity on the A-375 human melanoma cell line. Most of the tested deriva. were effective in decreasing cell proliferation, facilitating morphol. differentiation, and reprogramming gene expression. All these effects were reversable upon withdrawal of NT inhibitors. Among the compds. tested, 3f (I) showed the highest antiproliferative effect, whereas compound 6c, although not affecting cell proliferation, is endowed with a strong cytodifferentiating effect, which is probably related to a marked upregulation of the n-cad gene. These results support the potential of NNRTIs as valuable antitumor

IT 935480-63-0P
RLa RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(triazinones as regulators of cell differentiation and proliferation)

L4 ANSWER 5 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
RN 935480-63-0 CAPLUS
CN Benzenemethanimidamide, 2,6-difluoro-4-methyl- (CA INDEX NAME)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:174606 CAPLUS
DOCUMENT NUMBER: 146:251662
TITLE: Xanthine derivatives as selective HM74A agonists and their preparation
INVENTOR(S): Bailey, Richard Jonathan Daniel; Heer, Jag Paul; Liddle, John; Mason, Andrew Nemurtrie; Panto, Ivan Leo; Rahman, Shahzad Sharoogy Smith, Ian Edward David
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 312pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007027262	A1	20070215	WO 2006-EP7869	20060808
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
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AU 2006278216	A1	20070215	AU 2006-278216	20060808
CA 2618963	A1	20070215	CA 2006-2618963	20060808
EP 1912992	A1	20080423	EP 2006-776698	20060808
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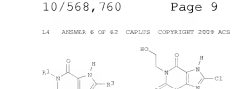
IN 2008MN00060	A	20080623	IN 2008-MN60	20080201
MX 2008001829	A	20080224	MX 2008-1829	20080208
KR 2008039396	A	20080506	KR 2008-705724	20080307
NO 2008001212	A	20080506	NO 2008-1212	20080307
CN 101163676	A	20080409	CN 2006-80037427	20080408
PRIORITY APPLN. INFO.:			GB 2005-16464	A 20050810
			GB 2006-7736	A 20060419
			GB 2006-14569	A 20060721
			WO 2006-EP7869	W 20060808

OTHER SOURCE(S): MARPAT 146:251662
GI

L4 ANSWER 6 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



AB The invention relates to compds. of formula I, which are xanthine derivs., processes for the manufacture of said derivs., pharmaceutical formulations containing the active compds. and the use of the compds. in therapy, for example, in the treatment of diseases where under-activation of the HM74A receptor contributes to the disease or where activation of the receptor will be beneficial. Compds. of formula I wherein R1 is (un)substituted C1-5 alkylene; R2 is H, (un)substituted C1-10 alkyl, (un)substituted C2-10 alkenyl, (un)substituted C2-10 alkynyl, (un)substituted cycloalkyl, (un)substituted cycloalkenyl, (un)substituted heterocyclyl, and (un)substituted (hetero)aryl; R3 is halo and CN; and their pharmaceutically acceptable derivs. thereof, are claimed. Example compound II was prepared by alkylation of 8-chloro-3-pentyl-7-(2-propen-1-yl)-3,7-dihydro-1H-purine-2,6-dione with 2-chlorowethanol followed by deallylation. All the invention compds. were evaluated for their HM74A agonistic activity.

IT 925444-92-3P 925444-98-0P
PL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of xanthine derivs. as selective HM74A agonists)

RN 925444-92-3 CAPLUS
CN Benzeneethaninidamide, 3-bromo-N-hydroxy-α,α-dimethyl-, [C(Z)]- (CA INDEX NAME)

Double bond geometry as shown.

RN 925444-98-0 CAPLUS
CN Benzeneethaninidamide, N,4-dihydroxy-α,α-dimethyl-, [C(Z)]-

L4 ANSWER 6 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

● Rf1

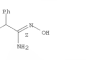
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
(CA INDEX NAME)

Double bond geometry as shown.

IT 42191-51-5 925698-75-5 925893-03-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of xanthine deriv. as selective HM74A agonists)

RN 42191-51-5 CAPLUS
CN Benzeneethaninidamide, N-hydroxy-α-methyl- (CA INDEX NAME)



RN 925698-75-5 CAPLUS
CN Benzeneethaninidamide, N-hydroxy-α-methyl-, [C(Z)]- (CA INDEX NAME)

Double bond geometry as shown.

RN 925893-03-4 CAPLUS
CN Benzeneethaninidamide, 4-chloro-N-hydroxy-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

Double bond geometry as shown.

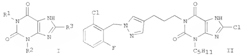
L4 ANSWER 7 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:176405 CAPLUS
DOCUMENT NUMBER: 146:251661
TITLE: Preparation of xanthine derivatives as selective HM74A agonists
INVENTOR(S): Hatley, Richard Jonathan Daniel; Mason, Andrew Nomuritis; Pinto, Ivan Leo
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 199pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007017261	A1	20070215	WO 2006-EP7865	20060808
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2006278215	A1	20070215	AU 2006-278215	20060808
CA 2626723	A1	20070215	CA 2006-2626723	20060808
EP 1912993	A1	20080423	EP 2006-763034	20060808
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
MX 2008001931	A	20080312	MX 2008-1931	20080208
IN 2008MN01117	A	20080711	IN 2008-MN1117	20080228
KR 2008003499	A	20080422	KR 2008-7005717	20080307
NO 2008002131	A	20080508	NO 2008-2131	20080327
CN 101163677	A	20080409	CN 2006-80037470	20080408
PRIORITY APPLN. INFO.:			GB 2005-16464	A 20050810
			GB 2006-7736	A 20060419
			GB 2006-14569	A 20060721
			WO 2006-EP7865	W 20060808

OTHER SOURCE(S): MARPAT 146:251661
GI

L4 ANSWER 7 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

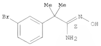


AB Xanthine derivs. of formula I [R1 = (CH2)mX(CH2)nY; X = heteroaryl, heterocyclyl; Y = (substituted) aryl, heteroaryl, aryloxy; m = 3-4; n = 0-1; R2 = (substituted) alkyl; R3 = halo] are prepared for the treatment of diseases where under-activation of the HM74A receptor contributes to the disease or where activation of the receptor will be beneficial. Thus, II was prepared from 3-pentyl-8-chloro-7-allyl-3,7-dihydro-1H-purine-2,6-dione, 4-(3-hydroxypropyl)pyrazole and 2-chloro-6-fluorobenzyl bromide. The prepared compds. had pEC50 values ≥ 4.3 and efficacy ≥ 30% in GTPγS binding assays.

IT 925444-91-3P 925444-98-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of xanthine derivs. as selective HM74A agonists)

RN 925444-91-3 CAPLUS
CN Benzeneethanimidamide, 3-bromo-N-hydroxy-α,α-dimethyl-, [C(Z)]- (CA INDEX NAME)

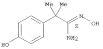
Double bond geometry as shown.



RN 925444-98-0 CAPLUS
CN Benzeneethanimidamide, N,4-dihydroxy-α,α-dimethyl-, [C(Z)]- (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 7 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

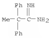
L4 ANSWER 8 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:30368 CAPLUS
DOCUMENT NUMBER: 146:317014
TITLE: New Optically Active N-Heterocyclic Carbene Complexes for Hydrogenation: A Tale with an Atropisomeric Twist
AUTHOR(S): Chen, Dianjun; Banphavichit, Vorawit; Reibenspies, Joe; Burgess, Kevin
CORPORATE SOURCE: Department of Chemistry, Texas A and M University, College Station, TX, 77843, USA
SOURCE: Organometallics (2007), 26(4), 855-859
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:317014

AB Iridium chiral 1,2,4-triazol-3-ylidene pyrimidine complexes derived from isoleucine were prepared and examined as catalysts for asym. hydrogenation of 1,2-diphenyl-1-propene; the complexes low enantioselectivity of 12% ee. Homologation and alkynylation of L-isoleucine afforded (3S,4R)-4-Boc-amino-3-methyl-7-dodecyn-6-one (8), which was condensed with amidines R(:NH)NH2 to give N-Boc-protected (αR)-2-R-6-Bu-α-[(1S)-1-methylpropyl]-4-pyrimidineethanamines (9a-c; R = Ph, 1-adamantyl, CMePh2). Deprotection of 9a-c followed by reaction with 3-(1-adamantyl)-1,3,4-oxadiazolium tetrafluoroborate gave the ligand precursors, 1-adamantyl-4-[(1R,2S)-1-(2-R-6-butyl-4-pyrimidinylmethyl)-2-methylbutyl]tetrazolium tetrafluoroborates (2a-c; R = Ph, 1-adamantyl, CMePh2), which upon metalation and halogen abstraction afforded the corresponding cationic iridium carbene-pyrimidine chelate cyclooctadiene complexes (5). A structure of the 1,2,4-triazolium salts is easily varied, allowing an access to a diverse set of N-heterocyclic carbene complexes. A coordinated chlorine atom was retained on reaction of 2 with [Ir(COD)Cl]2, and this resulted in two atropoisomeric complexes, 3 and 4, which were both characterized via x-ray diffraction studies. Neither of these complexes mediated hydrogenation of (E)-1,2-diphenyl-1-propene, but both 3 and 4 were reacted with NaBArF4 to give the chlorine-free complex 5, which was catalytically active in this reaction.

IT 173601-37-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of chiral carbene iridium triazolylidene-pyrimidine chelate complexes as catalysts for asym. hydrogenation of alkenes)

RN 173601-37-1 CAPLUS
CN Benzeneethanimidamide, α-methyl-α-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 8 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:199333 CAPLUS
DOCUMENT NUMBER: 146:229672
TITLE: Product subclass 4. 1-nitrogen-functionalized 1-haloalk-1-enes
AUTHOR(S): Rohanti, J. G.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2006), Volume Date 2005, 24, 223-264
CODEN: SCTCP9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review of methods to prepare 1-nitrogen-functionalized 1-haloalk-1-enes.
IT 40645-76-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(review preparation of nitrogen functionalized haloalkenes)
RN 40645-76-9 CAPLUS
CN Benzeneethanimidamide, N-[1-chloro-2-phenyl-1-propen-1-yl]-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

REFERENCE COUNT: 154 THERE ARE 154 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

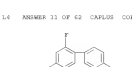
L4 ANSWER 10 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:951498 CAPLUS
DOCUMENT NUMBER: 144:467615
TITLE: Amidines (imidamides) N-substituted by metals, halogens, oxygen, and other heteroatoms
AUTHOR(S): Ostrowska, K.; Kolasa, A.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2005), 22, 489-563
CODEN: SCTCP9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review of the preparation and synthetic applications of amidine derivs.
IT 160154-90-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and synthetic applications of amidine derivs)
RN 160154-90-5 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, hydrazide (CA INDEX NAME)

REFERENCE COUNT: 838 THERE ARE 838 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:703874 CAPLUS
DOCUMENT NUMBER: 143:326018
TITLE: Synthesis and biological activity of flurbiprofen analogues as selective inhibitors of β-amyloid1-42 secretion
AUTHOR(S): Peretto, Ilaria; Radaelli, Stefano; Parini, Carlo; Sandi, Michele; Savegnia, Luca F.; Bonifo, Giulio; Fontanella, Laura; Mislano, Paola; Rigopoulos, Chiara; Rizzi, Andrea; Riccardi, Benedetta; Ricciardi, Marcello; Marchetti, Silvia; Puccini, Paola; Catinella, Silvia; Nondelli, Ivano; Cenacchi, Valentina; Bolzoni, Pier Tonino; Caruso, Paola; Villetti, Gino; Facchinetti, Fabrizio; Del Giudice, Elda; Moretto, Nadia; Imbimbo, Bruno P.
CORPORATE SOURCE: Research Development, Chiesi Farmaceutici S.p.A., Parma, 43100, Italy
SOURCE: Journal of Medicinal Chemistry (2005), 48(18), 5705-5720
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:326018
AB Flurbiprofen, a nonsteroidal antiinflammatory drug (NSAID), was recently described to selectively inhibit β-amyloid1-42 (Aβ42) secretion, the most toxic component of the senile plaques present in the brain of Alzheimer patients. The use of this NSAID in Alzheimer's disease (AD) is hampered by a significant gastrointestinal toxicity associated with cyclooxygenase (COX) inhibition. New flurbiprofen analogs were synthesized, with the aim of increasing Aβ42 inhibitory potency while removing anti-COX activity. In vitro ADME developability parameters were taken into account in order to identify optimized compds. at an early stage of the project. Appropriate substitution patterns at the alpha position of flurbiprofen allowed for the complete removal of anti-COX activity, while modifications at the terminal Ph ring resulted in increased inhibitory potency on Aβ42 secretion. In rats, some of the compds. appeared to be well absorbed after oral administration and to penetrate into the central nervous system. Studies in a transgenic mice model of AD showed that selected compds. significantly decreased plasma Aβ42 concns. These new flurbiprofen analogs represent potential drug candidates to be developed for the treatment of AD.
IT 884905-31-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. activity of flurbiprofen analogs as selective inhibitors of β-amyloid1-42 secretion devoid of anti-cyclooxygenase activity)
RN 884905-31-3 CAPLUS
CN [1,1'-Biphenyl]-4-ethanimidamide, 2-fluoro-N-hydroxy-α-methyl-4'-[(trifluoromethyl)- (CA INDEX NAME)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



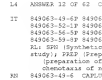
L4 ANSWER 12 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:283457 CAPLUS
DOCUMENT NUMBER: 142:355052
TITLE: Preparation of amidines and their salts useful in the inhibition of chemotaxis of neutrophils induced by interleukin-8
INVENTOR(S): Allegretti, Marcello; Cesta, Maria Candida; Nano, Giuseppe; Bertini, Riccardo; Bizzarri, Cinzia; Colotta, Francesco
PATENT ASSIGNEE(S): Dompe S.P.A., Italy
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005028425	A2	20050331	WO 2004-EP52201	20040916
WO 2005028425	A3	20050609		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004274183	A1	20050331	AU 2004-274183	20040916
CA 2539842	A1	20050331	CA 2004-2539842	20040916
EP 1667960	A2	20060607	EP 2004-787150	20040916
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1882539	A	20061220	CN 2004-80033491	20040916
JP 2007536286	T	20071220	JP 2006-527406	20040916
US 20070155717	A1	20070705	US 2006-568760	20060221
NO 20060172	A	20060419	NO 2006-172	20060119
PRIORITY APPLN. INFO.:			EP 2003-103557 A	20030925
			WO 2004-EP52201 W	20040916

OTHER SOURCE(S): CASREACT 142:355052; MARPAT 142:355052
AB Amidines ACR(CR3)C(=NR1)NR2 [A = (un)substituted Ph; benzoyl, (un)substituted heteroaryl; R = H, C1-5 alkyl, phenylalkyl, alkenyl, cycloalkyl, alkoxy, etc.; R1 = H, Me, Et; e.g., (E,S)-2-(4-isobutylphenyl)propionamidine hydrochloride], useful in the inhibition of chemotaxis of neutrophils induced by interleukin-8 in the treatment of psoriasis, ulcerative colitis, melanoma, chronic obstructive pulmonary disease, bullous pemphigus, rheumatoid arthritis, idiopathic fibrosis, glomerulonephritis, and in the prevention and treatment of damages caused by ischemia and reperfusion., are prepared

L4 ANSWER 12 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

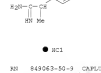
IT 849063-49-6P 849063-50-9P 849063-51-0P
849063-52-1P 849063-53-2P 849063-54-3P
849063-56-5P 849063-57-6P 849063-58-7P
849063-59-8P 849063-60-1P 849063-61-2P
RL: SPN (Synthetic preparation); TEM (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amidines and their salts useful in the inhibition of chemotaxis of neutrophils induced by interleukin-8)
RN 849063-49-6 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 849063-50-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, hydrochloride (1:1), (±)- (CA INDEX NAME)

Rotation (±).



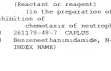
● HCl

RN 849063-51-0 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, hydrochloride (1:1), (-)- (CA INDEX NAME)

Rotation (-).

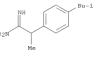
L4 ANSWER 12 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

IT 261178-48-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in the preparation of amidines and their salts useful in the inhibition of chemotaxis of neutrophils induced by interleukin-8)
RN 261178-48-7 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl-4-(2-methylpropyl)- (CA INDEX NAME)



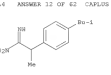
IT 849063-66-7P 849063-67-8P
RL: FOR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amidines and their salts useful in the inhibition of chemotaxis of neutrophils induced by interleukin-8)
RN 849063-66-7 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, (+)- (CA INDEX NAME)

Rotation (+).

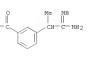


RN 849063-67-8 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, (-)- (CA INDEX NAME)

Rotation (-).

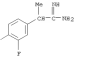


L4 ANSWER 12 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



● HCl

RN 849063-52-1 CAPLUS
CN Benzeneethanimidamide, 3-benzoyl-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



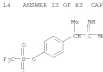
● HCl

RN 849063-53-2 CAPLUS
CN [1,1'-Biphenyl]-4-ethanimidamide, 2-fluoro-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 849063-54-3 CAPLUS
CN Methanesulfonic acid, 1,1,1-trifluoro-, 4-(2-amino-2-imino-1-methylethyl)phenyl ester, hydrochloride (1:1) (CA INDEX NAME)

L4 ANSWER 12 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

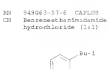


● HCl

RN 849067-56-5 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-[2-methylpropyl)-N-[3-[1-piperidinyl]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

● 2 HCl

RN 849063-53-6 CAPLUS
CN Benzeneethanimidamide, N,α-dimethyl-4-(2-methylpropyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

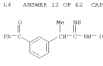
RN 849063-58-7 CAPLUS
CN Benzeneethanimidamide, 3-benzoyl-N-[3-(dimethylamino)propyl]-α-methyl-, hydrochloride (1:2) (CA INDEX NAME)

L4 ANSWER 12 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

RN 849063-61-2 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-N-(phenylmethyl)- (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

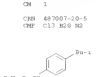


● 2 HCl

RN 849063-59-8 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

CRN 687007-20-5
CMF C13 H20 N2



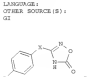
CM 2

CRN 64-19-7
CMF C2 H4 O2

RN 849063-60-1 CAPLUS
CN Benzeneethanimidamide, N-[3-(dimethylamino)propyl]-α-methyl-4-[2-methylpropyl]- (CA INDEX NAME)

L4 ANSWER 13 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:150032 CAPLUS
DOCUMENT NUMBER: 142:411301
TITLE: Inhibition of secretory phospholipase A2. 2-Synthesis and structure-activity relationship studies of 4,5-dihydro-3-(4-tetradecyloxybenzyl)-1,2,4-oxadiazol-5-one (PMS1062) derivatives specific for group II enzyme
AUTHOR(S): Dong, Chang-Zhi; Ahamada-Runidi, Araly; Plocki, Stephanie; Aoun, Darina; Touaibia, Mohamed; Meddad-Bel Habich, Nadia; Huet, Jack; Redeuilh, Catherine; Ombetta, Jean-Edouard; Godfroid, Jean-Jacques; Marsiot, Franc; Heymans, Francoise
CORPORATE SOURCE: Unite de Pharmacochimie Moleculaire et Systemes Membranaires (EA3381), Laboratoire de Pharmacochimie Moleculaire, Universite Paris 7-Denis Diderot, Paris, 75251, Fr.
SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(6), 1989-2007
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:411301
GI



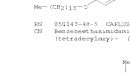
AB The discovery of a series of specific inhibitors of human group IIA phospholipase A2 (hGIIA PLA2) displaying promising in vitro and in vivo properties has been recently reported. Here the influence of different structural modifications on the specificity and potency of oxadiazolones, e.g. I [X = CH2, CH2CH2, CHMe, CMe2; R = MeO, n-octyloxy, n-tetradecyloxy, N,N-di(heptyl)amino, etc.], against hGIIA PLA2 vs. porcine group IB PLA2 is described. The SAR results, as well as the log P and pKa values of the oxadiazolones studied provide important information towards the comprehension of the mode of action of this kind of compds.

IT 310869-86-4P 850143-48-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and calculated hydrophobicity of ether, thioether or amino-functionalized aralkyl oxadiazolones as inhibitors of human secretory phospholipase A2 specific for group II enzyme)

RN 310869-86-4 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl-4-(tetradecyloxy)- (CA INDEX NAME)

L4 ANSWER 13 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

RN 852143-48-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-a,a-dimethyl-4-[(tetradecyloxy)- (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

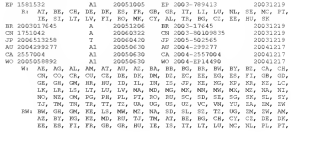
L4 ANSWER 14 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:550937 CAPLUS
DOCUMENT NUMBER: 141:106464
TITLE: Preparation of pyrazolo[3,4-b]pyridine derivatives for use in pharmaceutical compositions as phosphodiesterase inhibitors
INVENTOR(S): Allen, David George; Coe, Diane Mary; Cook, Caroline Mary; Cooper, William James; Nowle, Michael Dennis; Edlin, Christopher David; Hamblin, Julie Nicole; Johnson, Martin Redpath; Jones, Paul Spencer; Lindvall, Mika Kristian; Mitchell, Charlotte Jane; Rehrgruber, Allison Judith
PATENT ASSIGNEE(S): Cisco Group Limited, UK
SOURCE: PCT Int. Appl., 244 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056823	A1	20040708	WO 2003-EP14867	20031219
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
CA 2513349	A1	20040708	CA 2003-2513349	20031219
AU 2003293999	A1	20040714	AU 2003-293999	20031219
EP 1581532	A2	20051005	EP 2003-789413	20031219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
ER 200501764S	A	20051206	ER 2005-1764S	20031219
CN 1751042	A	20060322	CN 2003-80108935	20031219
JP 2006513258	T	20060420	JP 2005-502565	20031219
AU 2004299277	A1	20050630	AU 2004-299277	20041217
CA 2557004	A1	20050630	CA 2004-2557004	20041217
WO 2005058892	A1	20050630	WO 2004-EP14490	20041217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,

L4 ANSWER 14 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
SO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1737857	A1	20070103	EP 2004-804089	20041217
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV				
CN 1914205	A	20070214	CN 2004-80043657	20041217
JP 2007514764	T	20070607	JP 2006-544380	20041217
ZA 2005005074	A	20060927	ZA 2005-5074	20050622
IN 2005MN01207	A	20070713	IN 2005-MN1207	20050622
MX 2005PA06923	A	20050818	MX 2005-PA6923	20050623
NO 2005003690	A	20050824	NO 2005-3690	20050722
US 20062052790	A1	20061109	US 2006-540371	20060221
US 20070111965	A1	20070517	US 2006-596561	20060616
IN 2006MN01988	A	20070518	IN 2006-MN1988	20060714
NO 20060033440	A	20060918	NO 2006-3440	20060718
US 20080132536	A1	20080605	US 2008-22372	20080130
PRIORITY APPLN. INFO.:			GB 2002-30045	A 20021223
			GB 2002-30165	A 20021224
			GB 2003-7998	A 20030407
			WO 2003-EP14867	W 20031219
			GB 2004-5899	A 20040316
			GB 2004-5936	A 20040316
			GB 2004-6754	A 20040325
			WO 2004-EP14490	W 20041217
			US 2006-596561	A1 20060616

OTHER SOURCE(S): MARPAT 141:106464
GI



AB Pyrazolo[3,4-b]pyridine derivs., such as I [R = heterocyclyl; R1 = (CR2)2OR, alkyl, fluoroalkyl; R2 = H, Me, fluoroalkyl; R3 = alkyl, (un)substituted-Ph, cycloalkyl, heterocyclyl; R3a = H, alkyl], were prepared for therapeutic uses as inhibitors of phosphodiesterase, particularly phosphodiesterase IV (PDE4). These pyrazolo[3,4-b]pyridines were claimed for use in the treatment and/or prophylaxis of cognitive impairment and inflammatory and/or allergic diseases, such as chronic obstructive pulmonary disease (COPD), asthma, or allergic rhinitis. Thus, pyrazolo[3,4-b]pyridine derivative II was prepared via a cyclooxodesoxidation reaction of hydrazide III using POCl3 in MeCN. The prepared pyrazolo[3,4-b]pyridine were assayed for PDE4 inhibitory activity, and systems for delivery of these PDE4 inhibitors were discussed.

IT 925698-75-5
RL: PREP (Preparation)
(Preparation of pyrazolo[3,4-b]pyridine derivatives for use in pharmaceutical compositions as phosphodiesterase inhibitors)

RN 925698-75-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-a-methyl-, [C(S)]- (CA INDEX NAME)

Double bond geometry as shown.

IT 42191-51-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazolo[3,4-b]pyridine derivs. for use in pharmaceutical

L4 ANSWER 14 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
compds. as phosphodiesterase inhibitors)
RN 42191-51-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-a-methyl- (CA INDEX NAME)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

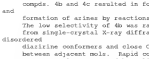
L4 ANSWER 15 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:275774 CAPLUS
DOCUMENT NUMBER: 138:368454
TITLE: Photochemistry of Crystalline Chlorodiazirines: The Influence of Conformational Disorder and Intermolecular Cl···H-N Interactions on the Solid-State Reactivity of Singlet Chlorocarbenes
AUTHOR(S): Sanrame, Carlos N.; Suhrada, Christopher P.; Sang, Rung; Garcia-Garibay, Miguel A.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California, Los Angeles, CA, 90095-1569, USA
SOURCE: Journal of Physical Chemistry A (2003), 107(10), 3287-3294
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:368454
AB A photochem. study was carried out with 3-R-substituted 3-chlorodiazirines with 4-biphenyl- (4a), (4-biphenyl)methyl- (4b), 2-(4-biphenyl)ethyl- (4c), and 1,1-dimethyl-2-(4-biphenyl)ethyl (4d) substituents. The chlorodiazirines were prepared from the corresponding amidines by a procedure involving oxidation with tert-Bu hypochlorite under phase-transfer catalysis. The crystalline nature of 4a-d was established by differential scanning calorimetric anal., which revealed melting endotherms prior to thermal decomposition Photochem. results in crystalline solids were analogous to those observed in solution, and the products were analyzed in terms of the corresponding singlet-state chlorocarbene intermediates (5a-d). Irradiation of 4a in solution and in crystals resulted in formation of azine N(Cl:CHR)2Cl2 9a (R = C6H4-g-Ph) by reaction of carbene 5a with its precursor. Equally selective, diaziridine 4d gave alkene Me2C:CH(C6H4-p-Ph) 6d as the only product by a 1,2-Ph migration from carbene 5d. In contrast, irradiation of compds. 4b and 4c resulted in formation of two alkenes by 1,2-H shifts and formation of azines by reactions of the carbenes with their precursors. The low selectivity of 4b was rationalized in terms of structural data from single-crystal X-ray diffraction anal., which revealed two disordered diaziridine conformers and close Cl···H contacts between adjacent mols. Rapid conformational equilibration in the solid state was also suggested by solid-state 13C CPMAS NMR. Similar structural effects are also postulated to account for the solid-state reactivity of 4c.
IT 524068-77-7
RL: RCT (Reactant); RACT (Reactant or reagent)

L4 ANSWER 13 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
PTC anion., the influence of conformational disorder and intermol. Cl···H-N interactions on the solid-state reactivity of singlet chlorocarbenes formed in photolysis of 3-chlorodiazirines)
RN 524068-77-7 CAPLUS
CN [1,1'-Biphenyl]-4-ethanimidamide, a,a-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:428975 CAPLUS
DOCUMENT NUMBER: 135:371498
TITLE: Evolution of anti-HIV drug candidates. Part 1: From a-Anilinophenylacetamide (a-APA) to imidoyl thiourea (ITU)
AUTHOR(S): Ludovici, D. W.; Kukla, M. J.; Groux, P. G.; Krishnan, S.; Andries, K.; de Bethune, M.-P.; Azijn, H.; Pauwels, R.; De Clercq, E.; Arnold, E.; Janssen, P. A.
CORPORATE SOURCE: J. Janssen Research Foundation, Spring House, PA, 19477, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(17), 2225-2228
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:371498
GI



AB Stemming from work on a previous clin. candidate, loviride, and other a-APA derivs., a new series of potent non-nucleoside reverse transcriptase inhibitors (NNRTIs) has been synthesized. The ITU analogs, which contain a unique diarylated imidoyl thiourea, e.g. (I), are very active in inhibiting both wild-type and clin. important mutant strains of HIV-1.
IT 374063-57-7
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and activity of imidoyl thioureas as non-nucleoside reverse transcriptase inhibitors)
RN 374063-57-7 CAPLUS
CN Benzeneethanimidamide, 2,6-dichloro-N-[[4-cyanophenyl]amino]thioxomethyl]-a-methyl- (CA INDEX NAME)

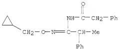
L4 ANSWER 16 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:265374 CAPLUS
DOCUMENT NUMBER: 134:280609
TITLE: Preparation of N-[α-(cyclopropylmethoximino)aralkyl]phenylacetamides and analogs as agrochemical fungicides
INVENTOR(S): Rheinheimer, Joachim; Eicken, Karl; Rose, Ingo; Grote, Thomas; Ammermann, Eberhard; Speakman, John-Bryan; Strathmann, Siegfried; Lorenz, Gisela
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

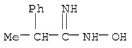
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001025187	A2	20010412	WO 2000-EP9744		20001005
WO 2001025187	A3	20011101			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2386513	A1	20010412	CA 2000-2386513		20001005
EP 1218339	A2	20020703	EP 2000-992195		20001005
EP 1218339	B1	20031001			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL					
JP 2003516933	T	20030520	JP 2001-528135		20001005
AT 251123	T	20031015	AT 2000-992195		20001005
TW 229662	B	20050321	TW 2000-89120773		20001005
US 6881742	B1	20050419	US 2002-89148		20020327
US 20050187265	A1	20050825	US 2005-61470		20050222
US 7101900	B2	20060905			
PRIORITY APPLN. INFO.:			DE 1999-19948266	A	19991006
			WO 2000-EP9744	W	20001005
			US 2002-89148	A3	20020327

OTHER SOURCE(S): MARPAT 134:280609
AB R1ZC(:NOR)NHCOR2 (R = cyclopropylmethyl)[I; R1 = (un)substituted Ph, -pyridyl, -thienyl; R2 = (un)substituted phenyl-, -thienyl-, -pyrazolylalkyl; Z = (un)substituted (heteroatom- or cyclopropylene-interrupted) alkylene] were prepared Thus, HONH2 was added

L4 ANSWER 17 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
to 2,6-Cl2C6H3CH2CN and the resulting amidoxime O-alkylated by cyclopropylmethyl bromide to give, after N-acylation, I (R1 = 2,6-Cl2C6H3, R2 = CH2Ph, Z = CH2). Data for biol. activity of I were given.
IT 333748-79-1P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-[α-(cyclopropylmethoximino)aralkyl]phenylacetamides and analogs as agrochem. fungicides)
RN 333748-79-1 CAPLUS
CN Benzeneacetamide, N-[1-[(cyclopropylmethoxy)amino]-2-phenylpropylidene]- (CA INDEX NAME)



IT 42191-51-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-[α-(cyclopropylmethoximino)aralkyl]phenylacetamides and analogs as agrochem. fungicides)
RN 42191-51-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl- (CA INDEX NAME)



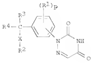
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:115148 CAPLUS
DOCUMENT NUMBER: 134:178571
TITLE: Preparation of 6-azauracil derivatives as interleukin-5 inhibitors
INVENTOR(S): Lacrampe, Jean Fernand Armand; Freyne, Eddy Jean Edgard; Deroose, Frederik Dirk; Fortin, Jerome Michel Claude; Coesemans, Erwin
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 163 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001010866	A1	20010215	WO 2000-EP7358		20000731
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2380759	A1	20010215	CA 2000-2380759		20000731
BR 2000013014	A	20020416	BR 2000-13014		20000731
EP 1206471	A1	20020522	EP 2000-948015		20000731
EP 1206471	B1	20060301			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL					
TR 200200310	T2	20020821	TR 2002-310		20000731
HU 2002002692	A2	20021228	HU 2002-2692		20000731
HU 2002002692	A3	20030128			
JP 2003506451	T	20030218	JP 2001-515675		20000731
EE 200200057	A	20030415	EE 2002-57		20000731
NZ 516506	A	20040227	NZ 2000-516506		20000731
CN 1188410	C	20050209	CN 2000-811339		20000731
AU 780047	B2	20050224	AU 2000-61609		20000731
AT 318811	T	20060315	AT 2000-948015		20000731
ES 2260031	T3	20061101	ES 2000-948015		20000731
TW 271404	B	20070121	TW 2000-89II5824		20000804
KR 795484	BI	20080116	KR 2002-700704		20020117
BG 106367	A	20020930	BG 2002-106367		20020130
IN 2002MN00144	A	20050318	IN 2002-MN144		20020131
NO 2002000565	A	20020326	NO 2002-565		20020205
NO 322386	B1	20060925			
ZA 2002001007	A	20030505	ZA 2002-1007		20020205
MX 2002PA01343	A	20020722	MX 2002-PA1343		20020206
US 20030114453	A1	20030619	US 2002-75876		20020214
US 6911444	B2	20050628			
HK 1048634	A1	20050930	HK 2003-100718		20030128
PRIORITY APPLN. INFO.:			EP 1999-870170	A	19990806
			EP 1999-126035	A	19991227

L4 ANSWER 18 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
WO 2000-EP7358 W 20000731

OTHER SOURCE(S): MARPAT 134:178571
GI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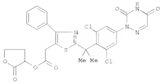
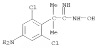

II

AB The title compds. (I) [p = 0-4; X = O, S, NR5, or a direct bond; or XR2 taken together = CN; R1 = independently C(O)ZR14, (un)substituted alkyl, halo, OH, SH, alkoxy, alkylthio, alkylcarbonyloxy, aryl, CN, NO2, hetercyclyl, R6, or NR7R8; R2 = heterocyclyl, (un)substituted cycloalkyl, alkoxy, or alkylthio, heterocyclyl(oxy), heterocyclylthio, etc.; R3 and R4 = independently H or (cyclo)alkyl; or R3 and R4 taken together form an alkenediyl; R5 = H or alkyl; R6 = (un)substituted (cyclo)alkylsulfonyl, amino(alkyl)sulfonyl, heterocyclylsulfonyl, etc.; R7 and R8 = independently H, (cyclo)alkyl, (di)hydroxyalkyl, mercaptoalkyl, aryl(alkyl), alkyloxyalkyl, alkyl(thio)carbonyl, aryl(thio)carbonyl, heterocyclyl(thio)carbonyl, C(O)ZR14, or (un)substituted aminocarbonyl, etc.; or R7 and R8 together with the N to which they are attached form a pyrrolinone, piperidinone, or hexahydroazepinone; R14 = H, alkynyl, or (un)substituted (alkyl)acyl, alkyl, alkenyl, heterocyclyl, etc.; Z = O, S, NH, CH2O, or CH2S; or ZR14 taken together = CH2CN or CH2PO3H2 and its esters] and their N-oxides, pharmaceutically acceptable salts, or stereochem. isomers were prepared as selective chemokine inhibitors. For example, 2,6-dichloro-4-(4,5-dihydro-3,5-dioxo-1,2,4-triazin-2(3H)-yl)-α,α-dimethylbenzeneethanethioamide was coupled with Et β-bromo-γ-oxobenzenebutanoate (46.5%), cyclized to form the

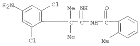
L4 ANSWER 18 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
thiazoleacetic acid (79%), and esterified with 3-bromodihydro-2(3H)-furanone to give II. As selective interleukin 5 (IL-5) and monocyte chemotactic protein-1 and -3 (MCP-1 and MCP-3) inhibitors, I are useful for treating eosinophil-dependent inflammatory diseases, esp. bronchial asthma (no data). Processes using I for marking receptors and imaging organs via radiolabeling are also claimed.

IT 261512-63-4P 325968-68-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of IL-5 inhibiting thiazolylalkylphenyl-6-azauracil derivs. by coupling of 4-dioxotriazinyl-α,α-dimethylbenzeneethanethioamides with α-oxoalkyl halides, cyclization, and addition of functionally substituted groups)

RN 261512-63-4 CAPLUS
CN Benzeneethanimidamide, 4-amino-2,6-dichloro-N-hydroxy-α,α-dimethyl- (CA INDEX NAME)



RN 325968-68-1 CAPLUS
CN Benzamide, N-[2-(4-amino-2,6-dichlorophenyl)-1-imino-2-methylpropyl]-2-methyl- (CA INDEX NAME)



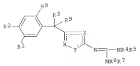
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:63983 CAPLUS
DOCUMENT NUMBER: 134:131527
TITLE: Preparation and effect of heteroaromatic ring compounds against autoimmune disorders and chronic inflammation
INVENTOR(S): Nakatsuka, Masashi; Nakatani, Shogo; Okada, Shin-ichiro; Tsuboi, Katsunori; Nishikaku, Fumio
PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan
SOURCE: PCT Int. Appl., 190 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001005774	A1	20010125	WO 2000-JP4616	20000710
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2377527	A1	20010125	CA 2000-2377527	20000710
EP 1201661	A1	20020502	EP 2000-944389	20000710
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
CN 1202095	C	20050518	CN 2000-810369	20000710
PRIORITY APPLN. INFO.:			JP 1999-201447 A	19990715
			JP 2000-58217 A	20000303
			WO 2000-JP4616 W	20000710

OTHER SOURCE(S): MARPAT 134:131527
GI

L4 ANSWER 19 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)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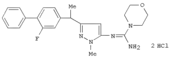
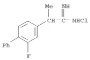

II

AB Title compds. [I; R1 = F, C6H5CO, C6H5CHO2(CH2)2; R2 = H, C6H5; R3 = H, CH3; R4 = H, CH3; R5 = CH3, CH2CH2N[(CH2)2]2O; R6 = H, CH3; R4-R5 = CH2CH2OCH2CH2, CH2CH2SCH2CH2, CH2CH2S(:O)(:O)CH2CH2; R6 = H, CH3; R7 = CH3, H, CH2CH2OH, CN, C(NH)N[(CH2)2]2O; R5-R7 = CH2CH2, CH2CH2CH2, CH2CHOHCH2; R6-R7 = CH2CH2OCH2CH2; R8 = H, CH3; R9 = H, CH3; X = N, NCH3, S; Y = NCH3, S, NH, NSO2C6H5; Z = CH, O, S, N; dotted line = single, double bond] and pharmaceutically acceptable salts exhibiting excellent phys. properties and potent ameliorative effects against both immune disorders and chronic inflammation are prepared. Thus, the title compound II was prepared and tested.

IT 321879-91-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and effect of heteroarom. ring compds. against immune disorders and chronic inflammation)

RN 321879-91-8 CAPLUS
CN [1,1'-Biphenyl]-4-ethanimidamide, N-chloro-2-fluoro-α-methyl- (CA INDEX NAME)



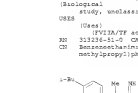
L4 ANSWER 39 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 40 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:900041 CAPLUS
DOCUMENT NUMBER: 134:137033
TITLE: FVIIA/TF activity inhibiting compounds
INVENTOR(S): Jakobsen, Palle; Persson, Egon
PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXU02
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000077046	A2	20001221	WO 2000-DK316	20000613
WO 2000077046	A3	20010222		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1192270	A2	20020403	EP 2000-934071	20000613
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003538839	T	20031021	JP 2001-503687	20000613
ES 2294430	T3	20080401	ES 2000-945577	20000613
US 6239078	B1	20010529	US 2000-614610	20000713
US 6444434	B1	20020903	US 2001-844028	20010427
US 20030073693	A1	20030417	US 2002-282826	20021002
PRIORITY APPLN. INFO.:			DK 1999-940	A 19990614
			US 1999-139714P	P 19990617
			DK 1999-910	A 19990625
			US 1999-141416P	P 19990629
			DK 1999-1241	A 19990903
			US 1999-152867P	P 19990908
			US 1999-141409P	P 19990629
			US 1999-141456P	P 19990629
			US 1999-141457P	P 19990629
			US 1999-141458P	P 19990629
			US 1999-141487P	P 19990629

L4 ANSWER 40 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
US 1999-141488P P 19990629
GB 1999-15597 A 19990702
US 1999-142724P P 19990708
US 1999-142725P P 19990708
US 1999-395492 A 19990914
US 1999-395851 A 19990914
US 1999-396657 A 19990921
US 1999-396660 A 19990921
US 1999-396661 A 19990921
US 1999-399855 A 19990915
US 2000-577731 B1 20000523
WO 2000-DK316 W 20000613
US 2000-614610 A1 20000713

AB The invention relates to compds. inhibiting the activation of FX to FXa by TF/FVIIa. The compds. are anticoagulants. The invention also relates to a method of identifying a drug candidate.
IT 313234-51-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(FVIIa/TF activity inhibiting compds.)
RN 313234-51-0 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-[2-methyl(propyl)-N-[2-[4-[2-methylpropyl]phenyl]propyl]- (CA INDEX NAME)



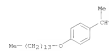
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 41 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:841977 CAPLUS
DOCUMENT NUMBER: 134:25351
TITLE: Heterocyclic phospholipase A2-specific inhibitors, their preparation, their use in treatment of inflammation, and pharmaceutical and cosmetic compositions containing them
INVENTOR(S): Assoqba, Leon; Reynaud, Francoise; Dong, Chang-Zhi; Godfroid, Jean-Jacques
PATENT ASSIGNEE(S): Universite Paris 7 - Denis Diderot, Fr.
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXU02
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000071138	A1	20001130	WO 2000-FR1386	20000519
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2793791	A1	20001124	FR 1999-6366	19990519
FR 2793791	B1	20020125		
PRIORITY APPLN. INFO.:			FR 1999-6366	A 19990519

OTHER SOURCE(S): MARPAT 134:25351
AB The invention provides phospholipase A2 inhibitor heterocyclic compds. (Markush included). The compds. are capable of acting on PLA2 and are advantageously secreted nonpancreatic PLA2-specific inhibiting compds. completely inactive towards pancreatic PLA2. The invention also provides a method for preparing the compds., pharmaceutical and cosmetic compns. containing them, and their use in particular for treating inflammatory pathologies.
IT 310869-84-4P
RL: ROT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction; heterocyclic phospholipase A2-specific inhibitor preparation, use in treatment of inflammation, and pharmaceutical and cosmetic compns. containing them)
RN 310869-84-4 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl-4-(tetradecyloxy)- (CA INDEX NAME)

L4 ANSWER 21 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L4 ANSWER 22 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:190770 CAPLUS
DOCUMENT NUMBER: 132:222555
TITLE: Preparation of interleukin-5 inhibiting 6-azauracil derivatives
INVENTOR(S): Freyne, Eddy Jean Edgard; Lacrampe, Jean Fernand Armand; Deroose, Frederik Dirk; Venet, Marc Gaston
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: Eur. Pat. Appl., 37 pp.
CODEN: EPXLDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 987265	A1	20000322	EP 1998-203148	19980910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CA 2344390	A1	20000330	CA 1999-2344390	19990914
WO 2000017195	A1	20000330	WO 1999-EP6776	19990914
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9960825	A	20000410	AU 1999-60825	19990914
AU 769133	B2	20040115		
EP 1114046	A1	20010711	EP 1999-947336	19990914
EP 1114046	B1	20030423		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002526495	T	20020820	JP 2000-574104	19990914
AT 238301	T	20030515	AT 1999-947336	19990914
ES 2198958	T3	20040201	ES 1999-947336	19990914
US 20020010177	A1	20020124	US 2001-812731	20010319
US 6594046	B2	20030715		
PRIORITY APPLN. INFO.:			EP 1998-203148 A	19980910
			WO 1999-EP6776 W	19990914

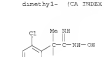
OTHER SOURCE(S): MARPAT 132:222555
GI

L4 ANSWER 22 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

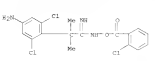
AB The title compds. [I; p = 0-4; X = O, S, NR5, SO2; R1 = alkyl, halo, polyhaloalkyl, etc.; R2 = Het1, cycloalkyl, alkyl, and if X = O, S, NR5, then R2 may also represent aminocarbonyl, aminothiocarbonyl, alkylcarbonyl, etc.; R3, R4 = H, alkyl, cycloalkyl; R3R4 = alkanediyl; R5 = H, alkyl; Het1 = (un)substituted heterocyclyl, useful for treating eosinophil-dependent inflammatory diseases, and naming a reagtor, were prepared and formulated. E.g., a multi-step synthesis of 3,8,4-trkaimn-3,5(2H,4H)-dione II which showed 90.5% inhibition of IL-5 production, was given.

IT 261512-63-4P 261512-64-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of interleukin-5 inhibiting 6-azauracil derivs.)

RN 261512-63-4 CAPLUS
CN Benzenesulfonimidamide, 4-amino-2,6-dichloro-N-hydroxy-N,4-dimethyl- (CA INDEX NAME)



RN 261512-64-5 CAPLUS
CN Benzoic acid, 2-chloro-, [2-[(4-amino-2,6-dichlorophenyl)-1-imino-2-methylpropyl]hexyl ester (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
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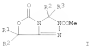
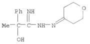
L4 ANSWER 22 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

L4 ANSWER 23 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:146378 CAPLUS
DOCUMENT NUMBER: 132:293711
TITLE: Synthesis of oxazolo[4,3-c]-1,2,4-triazol-5-ones
AUTHOR(S): Geffken, Detlef; Holst, Carsten; Willrodt, Imke
CORPORATE SOURCE: Institute of Pharmacy, Department of Pharmaceutical Chemistry, University of Hamburg, Hamburg, 20146, Germany
SOURCE: Heterocyclic Communications (2000), 6(1), 21-24
CODEN: HCOMEX; ISSN: 0793-0283
PUBLISHER: Freund Publishing House Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:293711
GI



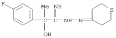
I

AB Treatment of 4-hydrazono-2-oxazolidinones with acetic anhydride afforded novel 2-acetyloxazolo[4,3-c]-1,2,4-triazol-5-ones (I; R1 = Me, H; R2 = Me, Ph, H, 4-fluorophenyl; CR2R3 = CHPh, cyclopentylidene, CMe2, CPh2, tetrahydropyran-4-ylidene, tetrahydrothiopyran-4-ylidene) in good yields.
IT 264124-05-2P 264124-09-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclic carbonylation of)
RN 264124-05-2 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, 2-(tetrahydro-4H-pyran-4-ylidene)hydrazide (CA INDEX NAME)

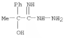


RN 264124-09-6 CAPLUS
CN Benzeneethanimidic acid, 4-fluoro-α-hydroxy-α-methyl-, 2-(tetrahydro-4H-thiopyran-4-ylidene)hydrazide (CA INDEX NAME)

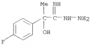
L4 ANSWER 23 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



IT 160154-90-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with tetrahydropyranone)
RN 160154-90-5 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, hydrazide (CA INDEX NAME)



IT 264124-07-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with tetrahydrothiopyranone)
RN 264124-07-4 CAPLUS
CN Benzeneethanimidic acid, 4-fluoro-α-hydroxy-α-methyl-, hydrazide (CA INDEX NAME)

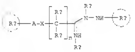


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1999:27808 CAPLUS
DOCUMENT NUMBER: 130:81527
TITLE: Preparation of novel amidrazone derivatives having antifungal activity
INVENTOR(S): Kageyama, Shunji; Kontani, Toru; Fujii, Masahiro; Igarashi, Kiyoshi; Yamamoto, Osamu
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9858905	A1	19981230	WO 1998-JP2817		19980624
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH, GW, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW					
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9879330	A	19990104	AU 1998-79330		19980624
PRIORITY APPLN. INFO.:			JP 1997-168354	A	19970625
			WO 1998-JP2817	W	19980624

OTHER SOURCE(S): MARPAT 130:81527
GI



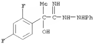
I

AB Amidrazone derivs. of formula [I; wherein the ring Ra represents: (1) an optionally substituted monocyclic to tricyclic aromatic hydrocarbon, (2) an optionally substituted monocyclic to tricyclic saturated or unsatd. hetero ring containing one or more hetero atoms selected from N, O and S, (3) an optionally substituted and optionally cross-linked cycloalkyl, or (4) an optionally substituted and optionally cross-linked cycloalkenyl; the ring Rb represents (1) an optionally substituted monocyclic to tricyclic aromatic hydrocarbon or (2) an optionally substituted monocyclic to tricyclic saturated or unsatd. hetero ring containing one or more hetero atoms selected from N, O and S; one of Rc and Rd represents H and the other is not present; Re

L4 ANSWER 24 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
represents H or OH; Rf represents H or lower alkyl, or YRa1; the dotted line "...." represents a single bond or a double bond; n is 1 to 8; A represents a bond or a lower alkylene optionally substituted by a lower alkyl; and X represents a bond, CO, CO2, CONRg, COCONRg1, CH:CHCONRg2, NRg3, NRg4CO, NRg5CO2, NRg6CONRg7, O, O2C, O2CNRg8, OCH2CONRg9, S, SO, SO2, SO2NRg10, or SO2NRg11CO; wherein Rg and Rg1 - Rg11 represent H, lower alkyl, or YRa2; Ra1 and Ra2 represents the same group as Ra; Y represents a single bond, CH2, or CO; a proviso given] or pharmaceutically acceptable salts thereof are prepd. Also claimed are pharmaceutical compns. thereof and a method for prevention or treatment of fungal or deep fungal infection by administration of I. These compds. I are useful for the treatment or prevention of fungal infection, in particular, deep fungal infection attributable to fungi, such as Candida, Aspergillus, and Cryptococcus. Thus, 2-(2-chloro-5-fluoro-6-oxo-1,6-dihydropyrimidin-1-yl)acetonitrile was treated with EtOH and HCl(g) in CHCl3 at 5° for 2 days to give a crude imidate which was condensed with 4-chlorophenylhydrazine hydrochloride in EtOH in the presence of EtONa at room temp. overnight to give the title compd., 2-pyrimidinyl-N-phenylacetamidrazone (II). II showed 80% min. inhibitory concn. of 0.31, 0.31, and 0.63 μg/mL against Candida albicans TIMM1768, Cryptococcus neoformans TIMM0362, and Aspergillus fumigatus TIMM1776, resp.
IT 218918-69-5P 218918-70-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel amidrazone derivs. having antifungal activity)
RN 218918-69-5 CAPLUS
CN Benzeneethanimidic acid, 2,4-difluoro-α-hydroxy-α-methyl-, 2-phenylhydrazide, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 218918-68-4
CMF C15 H15 F2 N3 O

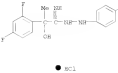


CM 2

CRN 144-62-7
CMF C2 H2 O4

L4 ANSWER 24 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

RN 228918-70-8 CAPLUS
CN Benzeneethanimidic acid, 2,6-difluoro-a-hydroxy-a-methyl-, 2-(4-chlorophenyl)hydrazide, hydrochloride (1:1) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

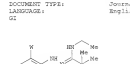
L4 ANSWER 25 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:573216 CAPLUS
DOCUMENT NUMBER: 129:196079
ORIGINAL REFERENCE NO.: 129:3967?a,3968a
TITLE: Racemic 2-Hydroxy-2-phenylpropanamidinium chloride and (S)-2-Hydroxy-2-phenylbutanamidinium (S)-2-Hydroxy-2-phenylethanoate
AUTHOR(S): Barnes, John C.; Weakley, Timothy J. R.
CORPORATE SOURCE: Dep. Chem., Univ. Dundee, Dundee, DD1 4HN, UK
SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (1998), C54(8), 1170-1173
CODEN: ACSCEY; ISSN: 0108-2701
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In 2-hydroxy-2-phenylpropanamidinium chloride, C9H13-N2O+.Cl-, the anion plays a central role in the H-bond network, chelating to one amidinium group and forming internol. links to neighboring NH2 and OH- groups. The central feature in (S)-2-hydroxy-2-phenylbutanamidinium (S)-2-hydroxy-2-phenylethanoate, C10H15N2O+.C8H7O3-, is a ring linking the cation and anion through two H bonds. The structure is extended by intra- and inter-mol. H bonds. Crystallog. data are given.
IT 92442-87-0
RL: PRP (Properties)
(crystal structure of)
RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, a-hydroxy-a-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:294826 CAPLUS
DOCUMENT NUMBER: 129:13472
ORIGINAL REFERENCE NO.: 129:2829a,2830a
TITLE: Amidoximes: a new class of coleopteran insecticides
AUTHOR(S): Futch, J. A.; Fuhr, D. G.; Hunt, David A.; Asselin, M.; Baffin, S. P.; Diehl, R. E.; Palmer, T. L.; Trotte, S. E.
CORPORATE SOURCE: Cyanamid Agric. Res. Cent., Am. Cyanamid Corp., Princeton, NJ, 08543-0400, USA
SOURCE: ACS Symposium Series (1998), 686(Synthesis and Chemistry of Agrochemicals V), 378-384
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

AB Amidoximes I [W = H, Cl, Br; X = H, CF3; Y = H, NO2, CF3; Z = H, Cl, Br, CF3, NO2] and related compds. were developed as insecticides specific against Coleoptera, especially Diabrotica undecimpunctata, with low toxicity to Lepidoptera, Acarina, fish, birds and mice. The synthesis of the compds. is outlined.
IT 156820-05-2 156820-27-8
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(insecticide specific against Coleoptera)
RN 156820-05-2 CAPLUS
CN Benzeneethanimidic acid, N-ethyl-a,a-dimethyl-, 2-[2,6-dichloro-4-(trifluoromethyl)phenyl]hydrazide (CA INDEX NAME)



RN 156820-27-8 CAPLUS
CN Benzeneethanimidic acid, 4-chloro-N-ethyl-a,a-dimethyl-, 2-[2,6-dichloro-4-(trifluoromethyl)phenyl]hydrazide (CA INDEX NAME)

L4 ANSWER 26 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1998:112229 CAPLUS
DOCUMENT NUMBER: 128:192667
ORIGINAL REFERENCE NO.: 128:38067a,38070a
TITLE: Preparation of substituted aromatic compounds as inhibitors of tumor necrosis factor and cyclic AMP phosphodiesterase
INVENTOR(S): He, Wei; Hulme, Christopher; Huang, Fu-chih; Djuric, Stevan W.; Moriarty, Kevin; Labaudiniere, Richard
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer Pharmaceuticals Inc., USA; He, Wei; Hulme, Christopher; Huang, Fu-Chih; Djuric, Stevan W.; Moriarty, Kevin; Labaudiniere, Richard
SOURCE: PCT Int. Appl., 154 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9805327	A1	19980212	WO 1997-US13343		19970722
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN					
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9738990	A	19980225	AU 1997-38990		19970722
PRIORITY APPLN. INFO.:			US 1996-23165P	P	19960805
			WO 1997-US13343	W	19970722

OTHER SOURCE(S): MARPAT 128:192667
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

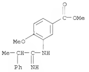
AB This invention is directed to compound of formula [I; ring A = Q10, Q11; Ar1 = Q12, Q13, Q14; ring Ar2 = (un)substituted fused Ph or fused monocyclic heteroaryl; R = (un)substituted alkyl, aralkyl, or heteroaralkyl, arylsulfonyl, heteroarylsulfonyl, etc.; R1 = carboxyalkyl, alkoxycarbonylalkyl, N-(un)substituted carbamoylalkyl, cyanoalkyl, (un)substituted aralkyl or heteroaralkyl; R2 = (un)substituted lower alkyl; R3 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, or oxaaliph., (un)substituted or optionally oxidized cyclothioalkyl or cyclothioalkenyl; R4, R6 = H, (un)substituted lower alkyl; R5 = (un)substituted alkyl, alkoxy, cycloalkyl, or heterocyclyl, alkoxycarbonyl, cyano, (un)substituted carbamoyl, (un)substituted aryl or heteroaryl, or CO_2H where m is other than 0; R7 = H, alkoxy,

(un)substituted cycloalkyl, cycloalkenyl, cycloalkoxy, cycloalkenyloxy, aryl, heteroaryl, aryloxy, heteroaryloxy, aralkyloxy, heteroaralkyloxy, alkylthio, or alkylsulfinyl, etc.; Q1, Q2 = CH_2, O-(un)substituted CHOH, CO; Q3, Q4, Q5, Q9 = N, optionally halo-substituted CH; Q6 = N, CH; Q7-C-Q8 = N-(un)satd. NHCH:N, O-CH:CH, CH:CH-O, O-CH_2CH_2, CH_2CH_2O; Z', Z'' = H or Z'Z'' = O or S; Z1, Z2 = direct bond, O, S; Z3 = SO_2, direct bond; Z4 = direct bond, O, S, NH; Z5 = direct bond, (un)substituted lower alkenyl; m, n = 0, 1; p = 1-3; q = 0-5] or hydrate, solvate, N-oxide, or prodrug thereof or a pharmaceutically acceptable salt thereof are They are esp. useful for inhibiting the prodn. or physiol. effects of tumor necrosis factor (TNF) and inhibit cAMP phosphodiesterase and are useful for the treatment of disease states assocd. with abnormally high physiol. levels of cytokines such as TNF or those assocd. with pathol. (e.g. asthma as bronchodilators or inflammation) conditions that are modulated by inhibiting enzymes such as cAMP phosphodiesterase (no data). In particular, they are used for treating a disease state capable of being modulated by inhibiting TNF, e.g., joint inflammation, arthritis, rheumatoid arthritis, rheumatoid spondylitis and osteoarthritis, sepsis, septic shock, gram neg. sepsis, toxic shock syndrome, acute respiratory distress syndrome, asthma, bone resorption diseases, reperfusion injury, graft vs. host reaction, allograft rejection malaria, myalgias, HIV, AIDS, cachexia, Crohn's disease, ulcerative colitis, pyresis, systemic lupus erythematosus, multiple sclerosis, type I diabetes mellitus, psoriasis, Behcet's disease, anaphylactoid purpura nephritis, chronic glomerulonephritis, inflammatory bowel disease, and leukemia. They are also used for treating a pathol. condition assocd. with a function of cAMP phosphodiesterase, eosinophil accumulation or function of the eosinophil, e.g., asthma, atopic dermatitis, urticaria, allergic rhinitis, psoriasis, rheumatic arthritis, ulcerative colitis, Crohn's disease, adult respiratory distress syndrome, diabetes insipidus, keratosis, dermatitis, cerebral senility, multiinfarct dementia, senile dementia, memory impairment assocd. with Parkinson's disease, cardiac arrest, stroke, and intermittent claudication. The present invention is also directed to their pharmaceutical use, pharmaceutical compns. contg. the compds., and methods of their prepn. Thus, 2-(3-cyclopentyloxy-4-methoxyphenyl)-5-hydroxymethyl-2-(4-pyridylmethyl)indan-1,3-dione was treated with NaH in THF, tosylated by tosyl chloride at 0° to room temp. for 2 h, and then condensed with 1-methylpiperazine in the K_2CO_3 in acetone at room temp. for 4 days the presence of K_2CO_3 in acetone to give the title compd., piperazinylmethylpyridylmethylindandione deriv. (II).

IT 201287-52-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted aromatic compds. as inhibitors of tumor necrosis factor and cAMP phosphodiesterase)

RN 201287-52-7 CAPLUS

CN Benzoic acid, 3-[(1-imino-2-phenylpropyl)amino]-4-methoxy-, methyl ester (CA INDEX NAME)



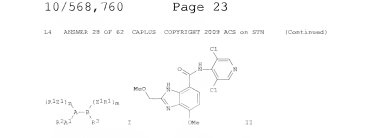
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1998:31305 CAPLUS
DOCUMENT NUMBER: 128:102087
ORIGINAL REFERENCE NO.: 128:20001a,20004a
TITLE: Substituted azabicyclic compounds and their use as inhibitors of the production of TNF and cyclic AMP phosphodiesterase
INVENTOR(S): Cox, Paul Joseph; Bower, Shelley; Aldous, David John; Astles, Peter Charles; McGarry, Daniel Gerard; Hulme, Christopher; et al.
PATENT ASSIGNEE(S): Regan, John Robinson, UK; Huang, Fu-Chih; Rhone-Poulenc Rorer Ltd.; Cox, Paul Joseph; Bower, Shelley; et al.
SOURCE: PCT Int. Appl., 355 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9748697	A1	19971224	WO 1997-GB1639		19970619
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW					
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
CA 2258728	A1	19971224	CA 1997-2258728		19970619
AU 9731026	A	19980107	AU 1997-31026		19970619
ZA 9705446	A	19981221	ZA 1997-5446		19970619
EP 934307	A1	19990811	EP 1997-926148		19970619
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI					
JP 2000509719	T	20000802	JP 1998-502503		19970619
US 6303600	B1	20011016	US 1998-216392		19981218
US 6800645	B1	20041005	US 2000-612530		20000707
US 20020173527	A1	20021121	US 2002-109629		20020328
US 20050038069	A1	20050217	US 2004-933077		20040901
US 7329675	B2	20080212			
PRIORITY APPLN. INFO.:			GB 1996-12760	A	19960619
			US 1996-23047P	P	19960802
			WO 1997-GB1639	W	19970619
			US 1998-216392	A1	19981218
			US 2000-612530	A3	20000707

OTHER SOURCE(S): MARPAT 128:102087
GI

L4 ANSWER 29 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



AB The invention is directed to physiol. active compds. of formula I |wherein
A2 = fused bicyclic ring system, of approx. 10-13 ring members, wherein A = azaheterocyclo ring and B = azaheteroaryl or optionally halo-substituted
benzene ring; R1 = H, (hydroxy- or halo-substituted) alkyl, and also alkenyl, alkynyl, or CHO when Z1 = bond; R2 = H, alkenyl, alkoxy, alkyl, aryl, aryloxy, cyano, etc.; R3 = wide variety of sidechains and functional
groups; A1 = bond, (un)substituted alkylene, alkenylene, alkynylene; Z1 = Bond, O, S, NH; n, n' = 0, 1; provided that (n+n) = 1] and their N-oxides, prodrugs, and pharmaceutically acceptable salts and solvates. I inhibit the production or physiol. effects of TNF, and inhibit cAMP phosphodiesterase
(PDE IV). The invention is also directed to pharmaceutical compns. comprising I, their pharmaceutical use, and methods for their preparation. For
instance, 7-methoxy-2-[methoxymethyl]-3H-benzimidazole-4-carboxylic acid [preparation given] was treated with O-benzotriazol-1-yl-N,N,N',N'-bis[tetramethylene]uronium tetrafluoroborate to give the 3-benzotriazolyl ester, which was amidated with 4-amino-3,5-dichloropyridine in THF (after treatment of the latter with Na diethylaluminate) to give the title compound
12. Compds. I had IC50 of 10-5 to 10-10 M against guinea pig macrophage PDE IV, with 50- to 10,000-fold selectivity for PDE IV vs. PDE I, II, III,
or V. The compds. also inhibited antigen-induced bronchoconstriction in rats by up to 89% at oral doses of 10 mg/kg.

IT 201287-52-7P

RL: BCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of azabicyclo compds. as inhibitors of TNF production and PDE IV)

RN 201287-52-7 CAPLUS

CN Benzoic acid, 3-[[1-imino-2-phenylpropyl]amino]-4-methoxy-, methyl ester (CA INDEX NAME)

L4 ANSWER 28 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 29 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:464218 CAPLUS
DOCUMENT NUMBER: 125:114673
ORIGINAL REFERENCE NO.: 125:21527a,21530a
TITLE: Preparation of benzyloxyphenylalkylbenzoates and related compounds as analgesics and prostaglandin antagonists
INVENTOR(S): Breault, Gloria Ann; Oldfield, John; Tucker, Howard; Warner, Peter
PATENT ASSIGNEE(S): Zeneca Limited, UK
SOURCE: PCT Int. Appl., 172 pp.
CODEN: PIXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9611902	A1	19960425	WO 1995-GB2417	19951012
W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
EA 9600622	A	19960912	EA 1995-9622	19951012
AU 9536162	A	19960506	AU 1995-36162	19951012
EP 737003	A1	19961025	EP 1995-937542	19951012
EP 737003	B1	19991222		
R: CH, DE, FR, GB, IT, LI				
JP 09511529	T	19971118	JP 1995-513027	19951012
US 5811459	A	19980922	US 1996-647977	19960604
PRIORITY APPLN. INFO.:			GB 1994-20557 A	19941012
			WO 1995-GB2417 W	19951012

OTHER SOURCE(S): MARPAT 125:114673
AB Ortho-substituted Ph, naphthyl, and heterocyclic ethers (> 600 compds.) were prepared for use in treating pain mediated by the E-type prostaglandins
(PGs data). Thus, 2-PhCH2OC6H4(CH2)2C6H4CO2R-4 was prepared from 2-HOC6H4Ac
and 4-OHC6H4CO2Me in 5 steps.

IT 179256-35-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzyloxyphenylalkylbenzoates and related compds. as analgesics and prostaglandin antagonists)

RN 179256-35-0 CAPLUS

CN Benzeneethanimidamide, α-methyl-2-(phenylmethoxy)- (CA INDEX NAME)

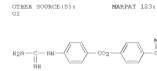
L4 ANSWER 29 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

L4 ANSWER 30 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:969831 CAPLUS
DOCUMENT NUMBER: 124:175546
ORIGINAL REFERENCE NO.: 124:32547a,32550a
TITLE: Conversion of 'obstinate' nitriles to amidines by Garigipati's reaction
AUTHOR(S): Moss, Robert A.; Ma, Wei; Merrer, Dina C.; Xue, Song
CORPORATE SOURCE: Dep. Chem., Rutgers, The State Univ. New Jersey, New Brunswick, NJ, 08903, USA
SOURCE: Tetrahedron Letters (1995), 36(48), 8761-4
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:175546
AB Reaction with methylchloroaluminum amide readily converts sterically hindered nitriles, e.g., 1-adamantanecarbonitrile, to amidines.
IT 177621-37-1P
RL: RPH (Synthetic preparation); PREP (Preparation)
(preparation of amidines by Garigipati amination of sterically hindered nitriles)
RN 177621-37-1 CAPLUS
CN Benzeneethanimidamide, α-methyl-α-phenyl- (CA INDEX NAME)

L4 ANSWER 31 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:678238 CAPLUS
DOCUMENT NUMBER: 123:55494
ORIGINAL REFERENCE NO.: 123:9903a,9904a
TITLE: Preparation of propionic acid derivatives as serine protease inhibitors
INVENTOR(S): Murakami, Motomi; Tamura, Toshiaki; Yanagi, Toshiharu
PATENT ASSIGNEE(S): Teikoku Chemical Industries Co. Ltd., Japan
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

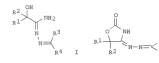
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9413623	A1	19940623	WO 1993-JP1783	19931209
W: JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 673924	A1	19951027	EP 1994-902692	19931209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:			JP 1992-360711	A 19921210
			JP 1993-318909	A 19931112
			WO 1993-JP1783	W 19931209

OTHER SOURCE(S): MARPAT 123:55494
GI



AB 2-[P-(p-guanidinobenzoyloxy)phenyl]propionic acid derivs. represented by general formula [I; A = OR, C1-6 lower alkoxy, NR1R2; C1-8 lower alkoxy which may be substituted by halogen, optionally substituted aryl, OCOR or succinimidoxy; R1, R2 = H, C1-8 lower alkyl, optionally substituted aralkyl or alternatively R1 and R2 are combined together with the adjacent nitrogen atoms to represent a heterocycle; B = OR, C1-8 lower alkyl, optionally substituted aryl, optionally substituted aryloxy, C1-8 lower alkoxy, optionally substituted aralkyloxy, NR1R2 (wherein R1 and R2 are each ar defined above)] or pharmaceutically acceptable acid-addition salts thereof is prepared. These compds. are useful as inhibitors of serine protease such as trypsin, chymotrypsin, plasmin, or thrombin and for the treatment of pancreatitis, bleeding, thrombosis, nephritis, and general

L4 ANSWER 32 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:22478 CAPLUS
DOCUMENT NUMBER: 122:81192
ORIGINAL REFERENCE NO.: 122:15427a,15430a
TITLE: 4-hydroxnooxazolidin-2-ones from α-substituted glycolamidrazones
AUTHOR(S): Geffken, D.; Holst, C.
CORPORATE SOURCE: Inst. Pharmazie, Universitaet Hamburg, Germany
SOURCE: Pharmazie (1994), 49(11), 821-4
CODEN: PHARAT; ISSN: 0031-7144
PUBLISHER: Govi-Verlag Pharmazeutischer Verlag
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 122:81192
GI



AB Hydrazinolysis of the glycolinidates gave glycolamidrazones which were with acetone or benzaldehyde to give hydrazono derivs. of type 4. I (R1 = alkyl, Ph, etc.; R2 = H, Me; R3 = Me, Ph, etc.; R4 = H, Me). Cyclic carbonylation of I with 1,1'-carbonyldiimidazole yields 4-hydrazono-2-oxazolidones II (same R1-R4).
IT 160154-90-5P, α-Hydroxy-α-methylbenzeneethanimidic acid hydrazide 160154-94-9P 160154-97-2P 160154-98-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (hydrazono)azolidinones from glycolamidrazones)
RN 160154-90-5 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, hydrazide (CA INDEX NAME)

RN 160154-94-9 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, 2-(1-methylethylidene)hydrazide (CA INDEX NAME)

L4 ANSWER 33 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
internal clot and prevention of blood coagulation under perfusion during dialysis or exchange of blood plasma. Thus, 3.44 g DCC was added to a mixt. of 3.85 g N,N-dimethylcarbamoylmethyl 2-(4-hydroxyphenyl)propionate, 3.00 g 4-guanidinobenzoic acid hydrochloride, and 20 mL pyridine and the resulting mixt. was stirred at room temp. overnight to give, after workup and acidification with MeSO3H, N,N-dimethylcarbamoylmethyl 2-(4-[4-guanidinobenzoyloxy]phenyl]propionate methanesulfonate, which in vitro showed IC50 of 1.4 × 10-7 and 1.9 × 10-8 M against trypsin and plasmin, resp. A tablet formulation contg. (S)-(+)-2.MeSO3H (A = C42F3) was prepd.
IT 159239-63-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [(guanidinobenzoyloxy)phenyl]propionic acid derivs. as serine protease inhibitors)
RN 159239-63-1 CAPLUS
CN Benzoic acid, 4-[aminoiminomethyl]amino]-, 4-(2-amino-1-methylethyl)phenyl ester, methanesulfonate (1:2) (CA INDEX NAME)

CM 1

CRN 159239-62-0
CMF C17 H19 N5 O2

CM 2

CRN 75-75-2
CMF C H4 O3 S

L4 ANSWER 33 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

RN 160154-97-2 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, 2-cyclopentylidenehydrazide (CA INDEX NAME)

RN 160154-98-3 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, 2-(phenylmethylene)hydrazide (CA INDEX NAME)

L4 ANSWER 33 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:492882 CAPLUS
DOCUMENT NUMBER: 121:292882
ORIGINAL REFERENCE NO.: 121:53704h,53705a,53707a
TITLE: Amidinoethyl derivative
INVENTOR(S): Muramatsu, Motomi; Tamura, Toshiaki; Yanagi, Toshiji
PATENT ASSIGNEE(S): Teikoku Hormone Mfg Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXLAP
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06228070	A	19940816	JP 1993-305706	19931208
PRIORITY APPLN. INFO.:			JP 1993-305706	19931208

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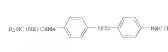


AB Amidinoethyl derivative I or its salts are useful as serine protease inhibitors for treatment of diseases (e.g. inflammation, cardiovascular diseases, and pancreatic diseases), caused by abnormalities of the enzyme. 4-[1-Amidinoethylphenol methanesulfonic acid salt (preparation given) (5.73 g) was stirred with 5.15 g 4-guanidinobenzoyl chloride HCl salt under ice cooling for 0.5 h and at room temperature overnight to give 3.76 g 4-(1-amidinoethylphenyl 4-guanidinobenzoate (II) dimethanesulfonate salt. II inhibited trypsin and thrombin with IC50 of 3.2 × 10-7 and 6.3 × 10-9 (no unit given).
IT 159239-62-0P 159239-63-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (amidinoethylphenyl guanidinobenzoate for inhibition of serine proteases)
RN 159239-62-0 CAPLUS
CN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[2-amino-2-imino-1-methylethyl]phenyl ester (CA INDEX NAME)

L4 ANSWER 33 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

RN 159239-63-1 CAPLUS
CN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[2-amino-2-imino-1-methylethyl]phenyl ester, methanesulfonate (1:2) (CA INDEX NAME)

CM 1

CRN 159239-62-0
CMF C17 H19 N5 O2

CM 2

CRN 75-75-2
CMF C H4 O3 S

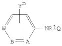
L4 ANSWER 34 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:502030 CAPLUS
DOCUMENT NUMBER: 121:102030
ORIGINAL REFERENCE NO.: 121:18219a,18222a
TITLE: N-arylhydrazine derivatives as insecticides and acaricides
INVENTOR(S): Furch, Joseph Augustus; Kuhn, David George; Hunt, David Allen; Law, Albert Chieh; Gronostajski, Cynthia Rena
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: Eur. Pat. Appl., 50 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 604798	A1	19940706	EP 1993-119754	19931208
EP 604798	B1	20020220		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
US 5420165	A	19950530	US 1992-998105	19921229
AT 213387	T	20020315	AT 1993-119754	19931208
ES 2173088	T3	20021016	ES 1993-119754	19931208
CZ 286479	B6	20000412	CZ 1993-2808	19931217
AU 9352679	A	19940714	AU 1993-52679	19931224
AU 675153	B2	19970130		
CA 2112420	C	20070213	CA 1993-2112420	19931224
RO 113556	B1	19980828	RO 1993-1796	19931227
SK 281733	B6	20010710	SK 1993-1484	19931227
IL 108188	A	20011125	IL 1993-108188	19931227
CN 1089938	A	19940727	CN 1993-121610	19931228
CN 1044600	C	19990811		
SA 9300740	A	19940818	SA 1993-9740	19931228
JP 06293685	A	19941021	JP 1993-350030	19931228
JP 3816543	B2	20060830		
NZ 250154	A	19941101	NZ 1993-250154	19931228
HU 67254	A2	19950328	HU 1993-3772	19931228
HU 215126	B1	20000628		
PL 175498	B1	19980128	PL 1993-317481	19931228
PL 174108	B1	19980430	PL 1993-301619	19931228
RU 2140708	C1	19991110	RU 1993-56649	19931228
CA 2112420	A1	19940630	CA 1994-2112420	19940121
US 5565589	A	19961217	US 1995-431227	19950428
US 5646276	A	19970708	US 1995-431154	19950428
US 5693860	A	19971202	US 1995-430031	19950428
JP 2005263809	A	20050929	JP 2005-134574	20050502
PRIORITY APPLN. INFO.:			US 1992-998104	A 19921229
			US 1992-998105	A 19921229
			JP 1993-350030	A3 19931228

OTHER SOURCE(S): MARPAT 121:102030
GI

L4 ANSWER 34 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



I

AB The N-arylhydrazine derivs. I [A,B,W=N,CR4;

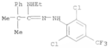
Y=halo,CN,NO2,(halo)alkyl,(halo)alkoxy;n=0,1,2;Q=NR2CRO,N:CRX1,N:CR(NR3R4); R=H,(halo)alkyl,cycloalkyl,(halo)alkoxy,etc.;R1,R2=H,alkyl; R3,R4=H,(un)substituted alkyl,Ph or pyridyl, etc.] are prepared as acaricides and insecticides. Treatment of 2,6-dichloro-4-(trifluoromethyl)phenylhydrazine with trimethylacetyl chloride, in Cl2CH2, gave 2,2-dimethylpropionic acid 2-(2,6-dichloro-α,α,α-trifluoro-p-tolyl)hydrazide (II). Lima bean leaves dipped in 300 ppm II were lethal to Southern armyworm (Spodoptera eridania) 3rd instar larvae.

IT 156820-05-2P 156820-21-2P 156820-27-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as acaricide and insecticide)

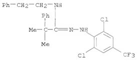
RN 156820-05-2 CAPLUS

CN Benzeneethanimidic acid, N-ethyl-α,α-dimethyl-, 2-[2,6-dichloro-4-(trifluoromethyl)phenyl]hydrazide (CA INDEX NAME)



RN 156820-21-2 CAPLUS

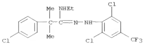
CN Benzeneethanimidic acid, α,α-dimethyl-N-(2-phenylethyl)-, 2-[2,6-dichloro-4-(trifluoromethyl)phenyl]hydrazide (CA INDEX NAME)



L4 ANSWER 34 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

RN 156820-27-8 CAPLUS

CN Benzeneethanimidic acid, 4-chloro-N-ethyl-α,α-dimethyl-, 2-[2,6-dichloro-4-(trifluoromethyl)phenyl]hydrazide (CA INDEX NAME)

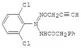


L4 ANSWER 35 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1991:6034 CAPLUS
DOCUMENT NUMBER: 114:6034
ORIGINAL REFERENCE NO.: 114:1187a,1190a
TITLE: Preparation of N-hydroxyamidines as acaricides and agricultural and horticultural fungicides
INVENTOR(S): Kishimoto, Takashi; Hayakawa, Koichi; Nakayama, Akira; Yamada, Tomio; Takahashi, Eiko; Hashimoto, Akira; Sano, Shinsuke; Hosokawa, Hiroyasu
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp. CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02006453	A	19900110	JP 1988-158393	19880627
PRIORITY APPLN. INFO.:			JP 1988-158393	19880627

OTHER SOURCE(S): MARPAT 114:6034
GI



III

AB Amidines R1[R5(R2O)N]C:NR3 (I) and R1(R3R4N)C:NOR2 II [R1 = H, (un)substituted Ph, alkyl optionally substituted by (un)substituted Ph, naphthyl, alkylthio, aralkylthio, (un)substituted NH2, cyclic amino, (un)substituted heterocyclyl; R2 = H, (un)substituted alkyl, alkenyl, alkynyl, XR6, X = CO, CONH, CO2, COCO; R6 = alkyl, (un)substituted alkenyl, Ph, or aralkyl, P(:Y)(OR7)2, Y = O, S, R7 = alkyl; R3 = H, (un)substituted alkyl, alkynyl, ZR8; Z = CO, CS, CO2, COCO, CONH, SO2, O2C; R8 = (un)substituted alkyl, alkenyl, or aralkyl, piperidino; R4 = H, alkyl; R5 = alkyl, aralkyl, (un)substituted aralkylcarbonyl] are prepared, e.g. by reaction of R1C(X):NOR2 (X = halo) with HNR3R4. Thus, PhCH2COCl was added to a solution of 2,6-Cl2C6H3C(NH2):NOCH2C.tplbond.CH in benzene and the mixture was refluxed overnight to give a benzamidine III. A total of 574 II were prepared and 18 II at 125 ppm completely controlled Tetranychus urticae and III and 46 others at 200 ppm controlled 77-100% Erysiphe graminis.

IT 129860-61-3P 129860-62-4P 129860-63-5P 129860-64-6P 129860-67-9P 129860-68-0P

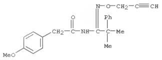
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

L4 ANSWER 35 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

(prepn. of, as acaricide and agrochem. fungicide)

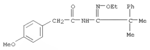
RN 129860-61-3 CAPLUS

CN Benzeneacetamide, 4-methoxy-N-[2-methyl-2-phenyl-1-[(2-propyn-1-yloxy)amino]propylidene]- (CA INDEX NAME)



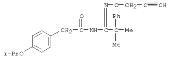
RN 129860-62-4 CAPLUS

CN Benzeneacetamide, N-[1-(ethoxyamino)-2-methyl-2-phenylpropylidene]-4-methoxy- (CA INDEX NAME)



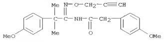
RN 129860-63-5 CAPLUS

CN Benzeneacetamide, 4-(1-methylethoxy)-N-[2-methyl-2-phenyl-1-[(2-propyn-1-yloxy)amino]propylidene]- (CA INDEX NAME)



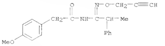
RN 129860-64-6 CAPLUS

CN Benzeneacetamide, 4-methoxy-N-[2-(4-methoxyphenyl)-2-methyl-1-[(2-propyn-1-yloxy)amino]propylidene]- (CA INDEX NAME)

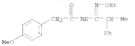


RN 129860-67-9 CAPLUS

L4 ANSWER 35 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
CN Benzeneacetamide, 4-methoxy-N-[2-phenyl-1-[(2-propyn-1-yloxy)amino]propylidene]- (CA INDEX NAME)



RN 129860-68-0 CAPLUS
CN Benzeneacetamide, N-[1-(ethoxyamino)-2-phenylpropylidene]-4-methoxy- (CA INDEX NAME)



L4 ANSWER 36 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1990:77194 CAPLUS
DOCUMENT NUMBER: 112:77194
ORIGINAL REFERENCE NO.: 112:13203a,13206a
TITLE: Preparation of oxadiazoles as central muscarinic acetylcholine receptor stimulants and pharmaceutical compositions containing them
INVENTOR(S): Baker, Raymond; Merchant, Kevin J.; Saunders, John; Street, Leslie J.
PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 323864	A2	19890712	EP 1989-200001	19890102
EP 323864	A3	19911218		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ZA 8900045	A	19900926	ZA 1989-45	19890104
DK 8900041	A	19890709	DK 1989-41	19890106
AU 8927798	A	19890720	AU 1989-27798	19890106
AU 628311	B2	19920917		
JP 02149580	A	19900608	JP 1989-571	19890106

PRIORITY APPLN. INFO.: GB 1988-394 A 19880108
GB 1988-13513 A 19880608
GB 1988-24898 A 19881024

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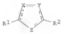
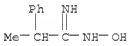
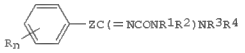

I

AB The title compds. [I; R1 = non-aromatic aza(bi)cyclic ring residue, e.g., pyrrolidinyl, piperidinyl, tetrahydropyridinyl; R2 = (substituted) saturated hydrocarbyl, e.g., Pr, Me2CH; one of X, Y, and Z = O and the other 2 = N], central muscarinic acetylcholine receptor stimulants, useful for treatment and prevention of neurodegenerative diseases, are prepared via cyclocondensation of R3CO2H with HON:CR4NH2 or R4CONHNH2 [one of R3 and R4 = non-aromatic aza(bi)cyclic ring residue and the other = (substituted) saturated

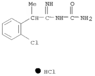
L4 ANSWER 36 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
hydrocarbyl]. PhCH2C(NH2):NOH was condensed with 3-(methoxycarbonyl)quinuclidine in THF contg. NaH to give 3-(3-benzyl-1,2,4-oxadiazol-5-yl)quinuclidine, isolated as its hemioxalate. A tablet comprising 3-(3-cyclopropyl-1,2,4-oxadiazol-5-yl)-1-azabicyclo[2.2.1]heptane 1.0, microcryst. cellulose 49.25, modified food corn starch 49.25, and Mg stearate 0.50 mg was formulated. I had an IC50 of better than 10 μM for displacement of specifically bound [3H]-N-methylscopolamine from muscarinic receptors of rat cortical membrane prepns.
IT 42191-51-5, 2-Phenylpropionamide oxime
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of oxadiazoles for treatment of neurodegenerative diseases)
RN 42191-51-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl- (CA INDEX NAME)



L4 ANSWER 37 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1981:480429 CAPLUS
DOCUMENT NUMBER: 95:80429
ORIGINAL REFERENCE NO.: 95:13591a,13594a
TITLE: Synthesis and properties of the tremor-inducing N-carbamoylacetamidine derivative LON-954 and some related compounds
AUTHOR(S): Bream, John B.; Picard, Claude W.; White, Trevor G.
CORPORATE SOURCE: Wander Res. Inst., Wander Ltd., Bern, CH-3001, Switz.
SOURCE: European Journal of Medicinal Chemistry (1981), 16(2), 175-9
CODEN: EJMCA5; ISSN: 0009-4374
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:80429
GI

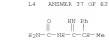

I

AB The hydration of N-cyanophenylacetamidines gave N-carbamoyl analogs I (Z = CH2, CHMe, CH2CH2, OCH2; Rn = H, Cl, Cl2; R1 = H, Me; R2 = H, Me; R3 = H, Me; R4 = H, Me). Thus, 2,6-Cl2C6H3CH2C(:NCN)NH2 was treated with concentrated HCl at 40-50° to give 2,6-Cl2C6H3CH2C(:NCONH2)NH2.HCl. The latter showed tremorogenic activity, while the other prepared I exhibited anti-tremorogenic activity.
IT 55769-76-1P 55769-91-0P 78622-01-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anti-tremorogenic activity of)
RN 55769-76-1 CAPLUS
CN Benzeneethanimidamide, N-(aminocarbonyl)-2-chloro-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



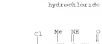
RN 55769-91-0 CAPLUS
CN Benzeneethanimidamide, N-(aminocarbonyl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

L4 ANSWER 37 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



● HCl

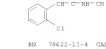
RN 78622-01-2 CAPLUS
CN Benzeneethanimidamide, N-(aminocarbonyl)-2,6-dichloro-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

IT 51770-09-7P 78622-11-4P 78630-47-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hydration of, N-carbamoylamidine analog from)
RN 51770-09-7 CAPLUS
CN Benzeneethanimidamide, 2-chloro-N-cyano-α-methyl- (CA INDEX NAME)

RN 78622-11-4 CAPLUS
CN Benzeneethanimidamide, N-cyano-α-methyl- (CA INDEX NAME)

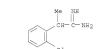


RN 78630-47-4 CAPLUS
CN Benzeneethanimidamide, 2,6-dichloro-N-cyano-α-methyl- (CA INDEX

L4 ANSWER 37 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

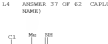
● HCl

RN 78622-24-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

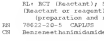


● HCl

L4 ANSWER 37 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



IT 78622-00-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with cyanogen bromide)
RN 78622-00-9 CAPLUS
CN Benzeneethanimidamide, 2,6-dichloro-α-methyl- (CA INDEX NAME)



IT 78622-19-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of cyanogen bromide with free base from)
RN 78622-19-2 CAPLUS
CN Benzeneethanimidamide, 2,6-dichloro-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

IT 55770-08-6 78622-24-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cyanogen bromide)
RN 55770-08-6 CAPLUS
CN Benzeneethanimidamide, 2-chloro-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

L4 ANSWER 38 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1978:406123 CAPLUS
DOCUMENT NUMBER: 89:6123
ORIGINAL REFERENCE NO.: 89:1043a,1046a
TITLE: O-(3-Amino-2-hydroxypropyl)amidoxime derivatives
INVENTOR(S): Takacs, Kalman; Nagy, Peter Listrati; Fisz, Ilona; Simay, Antal; Szentivanyi, Matyas; Virag, Sandor; Farago, Katalin
PATENT ASSIGNEE(S): Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt., Rumg.
SOURCE: Ger. Offen., 33 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2738589	A1	19780302	DE 1977-2738589	19770826
DE 2738589	C2	19900419		
HU 19948	A2	19810528	HU 1976-CI1682	19760827
HU 177578	B	19811128		
AT 7706054	A	19780815	AT 1977-6054	19770822
AT 355554	B	19800310		
SE 7709482	A	19780228	SE 1977-9482	19770823
SE 435280	B	19840917		
SE 435280	C	19841220		
NL 7709276	A	19780301	NL 1977-9276	19770823
NL 187479	B	19910516		
NL 187479	C	19911016		
IL 52804	A	19810629	IL 1977-52804	19770823
DD 132433	A5	19780927	DD 1977-200719	19770824
CH 2040008	B2	19810331	CH 1977-5551	19770824
GB 1580029	A	19801231	GB 1977-35745	19770825
BE 858134	A1	19771116	BE 1977-180647	19770826
DK 7707797	A	19780228	DK 1977-3797	19770826
DK 150196	B	19870105		
DK 150196	C	19870706		
FI 7702551	A	19780228	FI 1977-2551	19770826
FI 68396	B	19850531		
FI 68396	C	19850910		
NO 7702958	A	19780228	NO 1977-2958	19770826
NO 144793	B	19810907		
NO 144793	C	19811111		
FR 2362845	A1	19780324	FR 1977-26070	19770826
FR 2362845	B1	19810109		
JP 53050131	A	19780508	JP 1977-102504	19770826
JP 61016942	B	19870415		
AU 7728254	A	19790301	AU 1977-28254	19770826
AU 521432	B2	19820401		
PL 106317	B1	19791231	PL 1977-200400	19770826
PL 107628	B1	19800229	PL 1977-206476	19770826
HU 770296	A3	19900425	HU 1977-2514754	19770826
CA 1077506	A1	19800513	CA 1977-285529	19770826
CH 630244	A5	19820615	CH 1977-10477	19770826
US 4197220	A	19800205	US 1977-829148	19770830
CS 204009	B2	19810331	CS 1978-5952	19780914
AT 7808741	A	19800815	AT 1978-8741	19781207

L4 ANSWER 38 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

AT 361457	B	19810310			
US 4308399	A	19811229	US 1979-54791		19790705
PRIORITY APPLN. INFO.:			HU 1976-CI1682	A	19760827
			HU 1977-CI1682	A	19770426
			AT 1977-6054	A	19770822
			CS 1977-5551		19770824
			US 1977-829148	A3	19770830

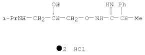
OTHER SOURCE(S): MARPAT 89:6123

AB RR1NCH2CH(OH)CH2ON:C(NH2)(CHR2)n(CHR3)mR4 I (R = H, C1-5 alkyl; R1 = C1-5 alkyl, cycloalkyl, Ph, optionally substituted by OH or Ph; RR1N = heterocycle; R2 = H, C1-4 alkyl, Ph; R3 = H, C1-4 alkyl, cycloalkyl or Ph, optionally substituted by halogen; R4 = optionally substituted cycloalkyl, aromatic or heterocyclic group; m = n = 0, 1, 2) and their salts were prepared. Thus, PhC(NH2):NOH reacted with 1-chloro-3-piperidino-2-propanol in EtOH to give I (RR1N = piperidino, R4 = Ph, m = n = 0). I are useful as antidiabetics.

IT 66611-55-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 66611-55-0 CAPLUS

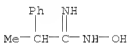
CN Benzeneethanimidamide, N-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]-α-methyl-, hydrochloride (1:2) (CA INDEX NAME)



IT 42191-51-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amines and epichlorohydrin)

RN 42191-51-5 CAPLUS

CN Benzeneethanimidamide, N-hydroxy-α-methyl- (CA INDEX NAME)



L4 ANSWER 38 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

L4 ANSWER 39 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1976:508660 CAPLUS
DOCUMENT NUMBER: 85:108660
ORIGINAL REFERENCE NO.: 85:17445a,17448a
TITLE: Pyrimidine derivatives
INVENTOR(S): Komori, Saburo
PATENT ASSIGNEE(S): Yanagida, Shozo, Japan
SOURCE: Jpn. Tokkyo Koho, 3 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 50037671	B	19751204	JP 1970-35552		19700425
PRIORITY APPLN. INFO.:			JP 1970-35552	A	19700425

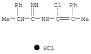
GI For diagram(s), see printed CA Issue.

AB Amidines I (R, R1 = Cl, alkyl, aralkyl, aryl) were heated with COCl2 to give pyrimidines II (R2 = Cl, OH). Thus, 2.3 g I (R = Cl, R1 = Me), 2.3 g COCl2, and PhCl were heated 90 hr in a sealed tube at 100-110° to give 2.01 g II (R = R2 = Cl, R1 = Me). Similarly prepared were II (R, R1, R2 given): Cl, Cl, OH; Cl, Ph, Cl; Me, Ph, Cl; Et, Et, Cl.

IT 40645-76-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with phosgene, pyrimidine derivative from)

RN 40645-76-9 CAPLUS

CN Benzeneethanimidamide, N-(1-chloro-2-phenyl-1-propen-1-yl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



L4 ANSWER 40 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1976:508659 CAPLUS
DOCUMENT NUMBER: 85:108659
ORIGINAL REFERENCE NO.: 85:17445a,17448a
TITLE: Barbituric acid derivatives
INVENTOR(S): Komori, Saburo
PATENT ASSIGNEE(S): Yanagida, Shozo, Japan
SOURCE: Jpn. Tokkyo Koho, 3 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 50037673	B	19751204	JP 1970-80192		19700912
PRIORITY APPLN. INFO.:			JP 1970-80192	A	19700912

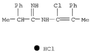
GI For diagram(s), see printed CA Issue.

AB Nitriles RCHR1CN (I) [R, R1 = (substituted) alkyl, Ph] or amides RCHR1CONH2 (II) were treated with COCl2 in the presence of HCl followed by treating the product with H2O to give III, which were also prepared by treating amidines IV (a mixture of cis and trans isomers) [R2, R3 = (substituted) alkyl, Ph] with COCl2 and then with H2O. Thus, 1.5 g IV.HCl (R - R3 = Me) and 2.4 g COCl2 in PhCl were heated in a sealed tube 20 hr at 100-110° to give 0.23 g III (R = R1 = Me), which was also prepared by heating a mixture of isobutyronitrile, HCl, COCl2 and PhCl in a sealed tube 77 hr at 100-110°. Similarly prepared were III (R, R1 given): Me, Et; Me, Ph; Bu, CH2CH2Br; Et, m-O2NC6H4.

IT 40645-76-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with phosgene)

RN 40645-76-9 CAPLUS

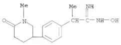
CN Benzeneethanimidamide, N-(1-chloro-2-phenyl-1-propen-1-yl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



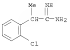
L4 ANSWER 41 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1976:30902 CAPLUS
DOCUMENT NUMBER: 84:30902
ORIGINAL REFERENCE NO.: 84:5045a,5048a
TITLE: Substituted α-phenylcarboxylic acids and their functional acid derivatives
INVENTOR(S): Rossı, Alberto
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Patentschrıft (Swıtz.), 6 pp. Dıvısıon of Swıss 559,173.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
CH 566311	A5	19750915	CH 1971-13160		19690605
PRIORITY APPLN. INFO.:			CH 1971-13160		19690605

GI For diagram(s), see printed CA Issue.
AB 4-[P-(1-carboxyethyl)phenyl]-5-(methylamino)valeric acid, prepared from 1-methyl-2-oxo-5-[p-(1-chloroethyl)phenyl]piperidine by treatment with NaCN, hydrolysıs, and ring cleavage, was cyclized to give the pıperıdınone
I. Antiinflammatory I was effective on rat paws in the Kaolin edema test ın oral doses of 30-100 mg/kg.
IT 41789-12-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparatıon of)
RN 41789-12-2 CAPLUS
CN Benzeneethanımıdamide, N-hydroxy-α-methyl-4-(1-methyl-6-oxo-3-piperidinyl)- (CA INDEX NAME)

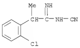


L4 ANSWER 42 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

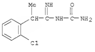


● HCl

IT 55770-09-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 55770-09-7 CAPLUS
CN Benzeneethanımıdamıde, 2-chloro-N-cyano-α-methyl- (CA INDEX NAME)



IT 55769-76-1P 55769-81-8P 55769-91-0P
55769-95-4P
RL: SPN (Synthetıc preparation); PREP (Preparation)
(preparation of, for antidepressants)
RN 55769-76-1 CAPLUS
CN Benzeneethanimidamide, N-(aminocarbonyl)-2-chloro-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

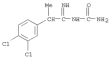
RN 55769-81-8 CAPLUS
CN Benzeneethanimidamide, N-(aminocarbonyl)-3,4-dichloro-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

L4 ANSWER 42 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1975:155896 CAPLUS
DOCUMENT NUMBER: 82:155896
ORIGINAL REFERENCE NO.: 82:24865a,24868a
TITLE: Aralıphatıc acetamidines
INVENTOR(S): Bream, John B.
PATENT ASSIGNEE(S): Dr. A. Wander, A.-G., Switz.
SOURCE: Ger. Offen., 28 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2439299	A1	19750306	DE 1974-2439299		19740816
FR 2241300	A1	19750321	FR 1974-27773		19740809
FI 7402392	A	19750221	FI 1974-2392		19740812
NO 7402887	A	19750221	NO 1974-2887		19740812
SE 7410281	A	19750221	SE 1974-10281		19740812
DK 7404280	A	19750428	DK 1974-4280		19740812
NL 7410987	A	19750224	NL 1974-10987		19740816
DD 116606	A5	19751205	DD 1974-180552		19740816
BE 818988	A1	19750219	BE 1974-147735		19740819
JP 50052043	A	19750509	JP 1974-94329		19740819
AU 7472496	A	19760219	AU 1974-72496		19740819
ZA 7405340	A	19760331	ZA 1974-5340		19740820
PRIORITY APPLN. INFO.:			GB 1973-39263	A	19730820
			GB 1973-44372	A	19730921

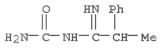
AB Thirty-three RnC6H5-nXC(:NR1)NHCONR2R3 (Rn = e.g. 3,4-Cl2, 3,4-Me2, 2-Cl, or 3-CF3; X = CH2, CHMe, or CH2CH2; R1-R3 = H or Me), useful as antidepressants, were prepared by hydrolysıs of RnC6H5-nXC(:NR1)NHCN or by
reaction of RnC6H5-nXC(:NR1)NH2 with R2NCO (R2 = e.g. Me) or with R2R3NCOCl.
IT 55770-08-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of)
RN 55770-08-6 CAPLUS
CN Benzeneethanimidamide, 2-chloro-α-methyl-, hydrochlorıde (1:1) (CA INDEX NAME)

L4 ANSWER 42 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



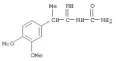
● HCl

RN 55769-91-0 CAPLUS
CN Benzeneethanimidamide, N-(aminocarbonyl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 55769-95-4 CAPLUS
CN Benzeneethanimidamide, N-(aminocarbonyl)-3,4-dimethoxy-α-methyl-, hydrochlorıde (1:1) (CA INDEX NAME)

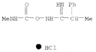


● HCl

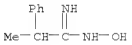
L4 ANSWER 43 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:466039 CAPLUS
DOCUMENT NUMBER: 79:66039
ORIGINAL REFERENCE NO.: 79:10667a,10670a
TITLE: Aromatic acetamidoxime O-carbamates
INVENTOR(S): Henderson, Rosetta M.
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co.
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 3742056	A	19730626	US 1971-135806		19710420
PRIORITY APPLN. INFO.:			US 1971-135806	A	19710420

AB Antihypertensive and antiinflammatory acetamidoxime O-carbamates, RnC6H5-nCHR1C(NH2):NO2CNHR2 (Rn = H, 4-Cl, 4-F, 2-Me, 4-NO2, 3,4-(MeO)2, 3,4-Me2, 2,4,6-Me3; R1 = H, Me; R2 = Me, Pr) were prepared by treating the acetamidoximes RnC6H5-nCHR1C(NH2):NOH with the isocyanates R2NCO.
IT 42191-44-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42191-44-6 CAPLUS
CN Benzeneethanimidamide, α-methyl-N-[[(methylamino)carbonyl]oxy]-, monohydrochloride (9CI) (CA INDEX NAME)



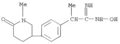
IT 42191-51-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with alkyl isocyanates)
RN 42191-51-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl- (CA INDEX NAME)



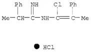
L4 ANSWER 44 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:418585 CAPLUS
DOCUMENT NUMBER: 79:18585
ORIGINAL REFERENCE NO.: 79:2983a,2986a
TITLE: Substituted α-phenylcarboxylicacids
INVENTOR(S): Rossi, Alberto
PATENT ASSIGNEE(S): Ciba-Geigy A.-G.
SOURCE: Patentschrift (Switz.), 7 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
CH 534680	A	19730430	CH 1972-3553		19690605
PRIORITY APPLN. INFO.:			CH 1972-3553	A	19690605

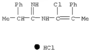
GI For diagram(s), see printed CA Issue.
AB The piperidinylphenylpropionic acids I [R = 1-acetyl-2(or 4)-piperidinyl, 1-methyl-2-oxo-4(or 5, or 6)-piperidinyl; R1 = H, Et] were prepared. Thus 4-(4-piperidinyl)phenylacetic acid was acetylated and then methylated with BuLi-MeI to I (R = 1-acetyl-4-piperidinyl, R1 = H). I were antiinflammatory at 30-100 mg/kg orally in the rat paw edema test.
IT 41789-12-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41789-12-2 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl-4-(1-methyl-6-oxo-3-piperidinyl)- (CA INDEX NAME)



L4 ANSWER 45 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:110501 CAPLUS
DOCUMENT NUMBER: 78:110501
ORIGINAL REFERENCE NO.: 78:17743a,17746a
TITLE: Nitrile salts. I. Dimerization of nitriles having α-hydrogen in the presence of hydrogen chloride
AUTHOR(S): Yanagida, Shozo; Fujita, Tetsuo; Ohoka, Masataka; Katagiri, Ichiro; Komori, Saburo
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(1), 292-9
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The compns. and structures of several stable nitrile HCl salts were investigated. Most were dimers and had the structure H2N+:C(CHRR2)NHCCl:CRR1.Cl-; hydrolysis gave HN(CONHRR1)2.
IT 40645-76-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40645-76-9 CAPLUS
CN Benzeneethanimidamide, N-(1-chloro-2-phenyl-1-propen-1-yl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



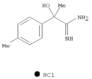
L4 ANSWER 46 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:97594 CAPLUS
DOCUMENT NUMBER: 78:97594
ORIGINAL REFERENCE NO.: 78:15663a,15666a
TITLE: Nitrile salts. II. Facile one-step synthesis of the pyrimidine nucleus
AUTHOR(S): Yanagida, Shozo; Fujita, Tetsuo; Ohoka, Masataka; Kumagai, Reiji; Komori, Saburo
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(1), 299-302
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The reaction of N-(α-chloroalkenyl)alkylamidine hydrochlorides (I) prepared from nitriles with two α-hydrogens reacted with COCl2 at 100-105° to give good yields of 4,6-dichloro-2,5-disubstituted-pyrimidines (II). I, which were obtained from nitriles with only one α-hydrogen, afforded 2-alkylidene-4,6-dichloro-5,5-disubstituted-2,5-dihydropyrimidines (III) in good yields.
IT 40645-76-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phosgene, pyrimidines by)
RN 40645-76-9 CAPLUS
CN Benzeneethanimidamide, N-(1-chloro-2-phenyl-1-propen-1-yl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



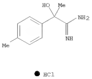
L4 ANSWER 47 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:84378 CAPLUS
DOCUMENT NUMBER: 78:84378
ORIGINAL REFERENCE NO.: 78:13469a,13472a
TITLE: Meso, racemic, and optically active forms of 3,6-bis[1-hydroxy-1-(4-methylphenylethyl]-1,2,4,5-tetrazines and related systems along with the corresponding 3,5-disubstituted 1,2,4-triazoles, their 4-amino derivatives, and 2,5-disubstituted 1,3,4-oxadiazoles including their circular dichroism spectra
AUTHOR(S): Neilson, D. G.; Mahmood, Safia; Watson, K. M.
CORPORATE SOURCE: Dep. Chem., Univ. Dundee, Dundee, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), (4), 335-9
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 78:84378
GI For diagram(s), see printed CA Issue.
AB (±)-, (+)-, (-)-, and meso-3,6-bis[1-hydroxy-1-(4-methylphenyl)-ethyl]-1,2,4,5-tetrazine (I) were prepared from the appropriate amidinium chlorides and H2NNH2.H2O. Reduction of I gave the corresponding 1,2-dihydrotetrazines (II) which rearranged in HCl-MeOH to give 4-amino-1,2,4-triazoles (III). Deamination of III with HNO2 gave 3,5-bis[1-hydroxy-1-(4-methylphenyl)ethyl]-1,2,4-triazoles. A mixture of meso- and (±)-I with MeCO3H gave 2,5-bis[1-hydroxy-1-(4-methylphenyl)ethyl]-1,3,4-oxadiazole. The 1-hydroxy-1-phenylethyl and 1-hydroxy-1-phenylpropyl analogs of I and II underwent similar reactions. The optically active compds. were studied by CD.
IT 941-50-4 941-51-5 941-52-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of)
RN 941-50-4 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

L4 ANSWER 47 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

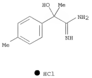


RN 941-51-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)



RN 941-52-6 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

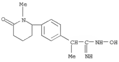


L4 ANSWER 48 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1971:405728 CAPLUS
DOCUMENT NUMBER: 75:5728
ORIGINAL REFERENCE NO.: 75:951a,954a
TITLE: α-Phenyl carboxylic acid compounds
INVENTOR(S): Rossi, Alberto
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: Ger. Offen., 98 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2025518	A	19701210	DE 1970-2025518		19700526
CH 559173	A5	19750228	CH 1969-8650		19690605
CH 573909	A5	19760331	CH 1970-6221		19700424
CA 980783	A1	19751230	CA 1970-83721		19700526
US 3801581	A	19740402	US 1970-41107		19700527
ZA 7003642	A	19710127	ZA 1970-3642		19700528
FR 2052932	A5	19710416	FR 1970-20213		19700602
FR 2052932	A1	19710416			
BE 751451	A	19701204	BE 1970-751451		19700604
NL 7008158	A	19701208	NL 1970-8158		19700604
GB 1319251	A	19730606	GB 1970-27284		19700605
GB 1319252	A	19730606	GB 1972-55884		19700605
US 3853892	A	19741210	US 1973-338698		19730307
PRIORITY APPLN. INFO.:			CH 1969-8650	A	19690605
			CH 1969-18441	A	19691211
			CH 1970-6221	A	19700424
			CH 1969-6221	A	19700424
			US 1970-41107	A2	19700527

AB Title compds., useful as anti-inflammatory agents, have the structure AC6H4CR1R2X, in which A = azacycloalkyl or -alkenyl, R1 and R2 are H or alkyl, and X = CO2H or a derivative Thus, 4-phenylpiperidine treated with C5H5N and AcCl give 1-acetyl-4-phenylpiperidine (I). I, AcCl, and CS2 is treated with AlCl3 to give 1-acetyl-4-(p-acetylphenyl)piperidine (II). II reduced with NaBH4 gives 1-acetyl-4-[p-(1-hydroxyethyl)phenyl]piperidine (III). SOCl2 converts III into 1-acetyl-4-[p-(1-chloroethyl)phenyl]piperidine, which is treated with NaCN to give 1-acetyl-4-[p-(1-cyanoethyl)phenyl]piperidine (IV). IV and aqueous ethanolic KOH, then HCl gives the HCl salt of α-[p-(4-piperidyl)phenyl]propionic acid, which is converted to its Et ester (V), then acetylated to give ethyl α-[p-(1-acetyl-4-piperidyl)phenyl]propionate, hydrolysis of which gives α-[p-(1-acetyl-4-piperidyl)phenyl]propionic acid. IV was similarly prepared from 2-(p-bromophenyl)-2-methyl-1,3-dioxolane Grignard reagent and 1-benzyl-4-piperidone via 2-[p-(1-benzyl-4-hydroxy-4-piperidyl)phenyl]-2-methyl-1,3-dioxolane,

L4 ANSWER 48 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
p-(1-benzyl-1,2,5,6-tetrahydro-4-pyridyl)acetophenone, and 1-hydroxy-1-[p-(4-piperidyl)phenyl]ethane. 1-Methyl-2-oxo-5-[p-(1-cyanoethyl)phenyl]piperidine is treated with NH2OH.HCl to give α-[p-(1-methyl-2-oxo-5-piperidyl)phenyl]propionamidoxime. p-(1-Acetyl-4-piperidyl)acetophenone, morpholine, and S react to give p-(1-acetyl-4-piperidyl)phenylthioacetic acid morpholide, which is hydrolyzed to p-(4-piperidyl)phenylacetic acid-HCl.
IT 32262-02-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 32262-02-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl-4-(1-methyl-6-oxo-2-piperidinyl)- (CA INDEX NAME)

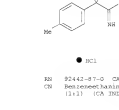


L4 ANSWER 49 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:42424 CAPLUS
DOCUMENT NUMBER: 70:42424
ORIGINAL REFERENCE NO.: 70:7975a,7976a
TITLE: Optical rotatory dispersion of α-hydroxy amidines and their transition metal complexes
AUTHOR(S): Neilson, Douglas G.
CORPORATE SOURCE: Univ. St. Andrews, Dundee, UK
SOURCE: Some Newer Phys. Methods Struct. Chem., Proc. Symp. (1967), Meeting Date 1966, 186-91. Editor(s): Bonnett, R. United Trade Press Ltd.: London, Engl. CODEN: 30LRAG
DOCUMENT TYPE: Conference
LANGUAGE: English
CC For diagram(s), see printed CA Issue.
AB O.R.D. of mandelanidinium chlorides (I) and lactamidinium chloride (II) were measured in MeOH or EtOH to obtain their absolute configuration, but the results were rather irregular; no full Cotton effect curves could be measured for (-)-I [R = H, 2-Cl, and 2-Br] and (-)-II, while 2 extrema were observed for (+)-I [3-MeO, 2-EtO, 4-MeO and 4-EtO]. Thus, O.R.D. of the Cu complexes were measured: all the Cu complexes of α-hydroxyamidines of known D-configuration exhibited a pos. Cotton effect, which permitted the D-configuration to be assigned to I [2-MeO, 2-EtO, 2-Cl, 2-Br, 4-MeO, 4-EtO, 3-EtO and 2,4-di-Cl] for which chemical methods cannot be applied owing to the facile racemization. The Cu complex of D-(+)-I gave a pos. O.R.D. curve, establishing the greater value of O.R.D. curves of Cu complexes over that of the parent amidines for the correlation of configuration. The Ni complex is also effective but proved difficult to synthesize. O.R.D. curves of some of the Cu complexes of I [2-EtO, 3-EtO and 4-MeO] have an addnl. extrema near 270 mμ. The Cotton effect owing to the ligand is counterbalanced by an effect of opposite sign but approx. equal intensity owing to the complex as a whole. Support for this argument was given by comparing the circular dichroism curves of I [2-Cl] and I [2-EtO] and their Cu complexes. O.R.D. of compds. containing the amidine group in a heterocyclic ring (e.g., imidazoline) are also discussed.
IT 22210-97-5
RL: PROC (Process)
(optical rotary dispersion of)
RN 22210-97-5 CAPLUS
CN Mandelanidine, α-methyl-, monohydrochloride, (+)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 50 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:454040 CAPLUS
DOCUMENT NUMBER: 63:54040
ORIGINAL REFERENCE NO.: 63:9794a-e
TITLE: Optical rotatory dispersion. XIX. A series of acids, imidazolines, amidinium chlorides, and their cupric complexes, related to mandelic acid
AUTHOR(S): Emerson, T. R.; Ewing, D. F.; Klyne, W.; Neilson, D. G.; Peters, D. A. V.; Roach, L. H.; Swan, R. J.
CORPORATE SOURCE: Univ. London, Swed.
SOURCE: Journal of the Chemical Society (1965), (July), 4009-14
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The optical rotatory dispersion (o.r.d.) curves of series of α-hydroxy acids related to mandelic acid show that the Cotton-effect curves observed are generally due to the n → π* transition of the carboxyl group and not to the phenyl absorption band (260-280 mμ). The o.r.d. curves for the related amidinium chlorides show distinct extrema in the 250-280 mμ region when the phenyl group carries an alkoxy-substituent. The o.r.d. curves of the amidinium chlorides, however, are more complex than those of their parent acids and not so useful for configurational assignments. Cu complexes derived from these α-hydroxyamidinium chlorides show a Cotton effect at .apprx.590 mμ. Compds of D-configuration have a positive Cotton effect in this region. This rule has permitted the assignment of configuration to some 10 amidines, not previously correlated by chemical means.
IT 941-52-6 92442-87-0
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 941-52-6 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, [-]- (9CI) (CA INDEX NAME)

Rotation (-).



● HCl

RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

L4 ANSWER 49 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

● HCl

L4 ANSWER 50 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

● HCl

IT 941-51-5, Mandelamidine, p,α-dimethyl-, hydrochloride, D-(-)- 4023-95-4, Mandelamidine, α-methyl-, hydrochloride, D-(-)- 94281-37-5, Mandelamidine, α,4-dimethyl-, hydrochloride, D-(-)-
(optical rotatory dispersion and spectrum of)
RN 941-51-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 4023-95-4 CAPLUS
CN Mandelamidine, α-methyl-, hydrochloride, D-(-)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 94281-37-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,3-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

L4 ANSWER 50 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

● HCl

L4 ANSWER 51 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:454039 CAPLUS
DOCUMENT NUMBER: 63:54039
ORIGINAL REFERENCE NO.: 63:9783h,9784a
TITLE: Optical rotatory dispersion. XV. Monosubstituted succinic acids
AUTHOR(S): Fredga, Arj. Jennings, J. F.; Klyne, W.; Scopes, Patricia M.; Sjoberg, B.; Sjoberg, S.
CORPORATE SOURCE: Univ. Uppsala, Swed.
SOURCE: Journal of the Chemical Society (1965), (July), 3926-35
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. CA 62, 13191g; 63, 9265g. The ORD curves of many α-substituted succinic acids are measured. All these compds. show Cotton effects associated with the carbonyl absorption band at about 225 mμ. α-Alkyl-, α-aryl-, and α-halosuccinic acids of the D-configuration all give pos. Cotton effects in water and in MeOH; D-α-Alkylthiosuccinic acids give somewhat more complex pos. curves. D-α-Hydroxysuccinic acid (D-malic acid) and its O-alkyl ethers give neg. Cotton effects in water and in MeOH. The signs of the dispersion curves of most of these acids are reversed on the addition of alkali.
IT 941-51-5 941-52-6 92442-87-0
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 941-51-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 941-52-6 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

L4 ANSWER 51 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

● HCl

RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

L4 ANSWER 52 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:66553 CAPLUS
DOCUMENT NUMBER: 62:66553
ORIGINAL REFERENCE NO.: 62:11822e-h,11823a-e
TITLE: 1,2,4-Oxadiazoles with pharmaceutical effect
INVENTOR(S): Harsanyi, Kalman; Kiss, Faj; Korosnits, Dezso; Malyata, Ilona; Erdelyi, Ilona; Tardos, Laszlo; Laszkovszky, Gyorgy
PATENT ASSIGNEE(S): Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt.
SOURCE: 23 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
HU 151748		19641223	HU	19630329
BE 645822			BE	
NL 302339			NL	
US 3280122		19661018	US 1964-354465	19640324
PRIORITY APPLN. INFO.:			HU	19630329

OTHER SOURCE(S): MARPAT 62:66553
AB A mixture of 24 g. β,β-diphenylpropionamidoxime(I), 37 g. Et β-piperidinopropionate, 200 ml. absolute EtOH, and 2.3 g. Na is refluxed 9 hrs., concentrated in vacuo, 200 ml. H2O and 4.0 g. NaOH are added, and the mixture is extracted with CHCl3. The organic phase is concentrated in vacuo and treated with 100 ml. EtOH-HCl to precipitate 29.22 g. 3-[β,β-diphenylethyl]-5-[β-piperidinoethyl]-1,2,4-oxadiazole-HCl, m. 192-3° (EtOH). Similarly are prepared the following derivs.: 3-[β,β-diphenylethyl]-5-[β-pyrrolidinoethyl]-1,2,4-oxadiazole N malonate, m. 129-31° (H2O or EtOAc), 3-[β,β-diphenylethyl]-5-(piperidinomethyl)-1,2,4-oxadiazole-HCl, m. 188-9°, 3-[β,β-diphenylethyl]-5-[β-diethylaminoethyl]-1,2,4-oxadiazole-HCl, m. 181°, 3-[β,β-diphenylethyl]-5-(4-aminophenyl)-1,2,4-oxadiazole, m. 145° (96% EtOH), 3-[β,β-diphenylethyl]-5-(4-pyridyl)-1,2,4-oxadiazole, m. 158-9°, 3-[β,β-diphenylethyl]-5-(3-pyridyl)-1,2,4-oxadiazole, m. 137°, 3-[β,β-diphenylethyl]-5-[2-pyridyl]-1,2,4-oxadiazole, m. 151-2°, 3-[α,β-diphenylethyl]-5-[β-piperidinoethyl]-1,2,4-oxadiazole-HCl, m. 183°, 3-diphenylmethyl-5-piperidinomethyl-1,2,4-oxadiazole-HCl, m. 161°, 3-diphenylmethyl-5-[β-piperidinoethyl]-1,2,4-oxadiazole-HCl, m. 197°, 3-(3,4-dimethoxyphenyl)-5-[β-morpholinoethyl]-1,2,4-oxadiazole-HCl, m. 181°, 3-(3,4-dimethoxyphenyl)-5-[β-pyrrolidinoethyl]-1,2,4-oxadiazole-HCl, m. 162°, 3-(3,4-dimethoxyphenyl)-5-[β-piperidinoethyl]-1,2,4-oxadiazole-HCl, m. 177°, 3-(3,4-dimethoxyphenyl)-5-piperidinomethyl-1,2,4-oxadiazole-HCl, m. 159°, 3-benzyl-5-[β-morpholinoethyl]-1,2,4-oxadiazole-HCl, m. 173°, 3-benzyl-5-[β-pyrrolidinoethyl]-1,2,4-oxadiazole-HCl, m. 156°, 3-[p-chlorobenzyl]-5-[β-piperidinoethyl]-1,2,4-oxadiazole-HCl, m. 183°, 3-[p-chlorobenzyl]-5-[β-morpholinoethyl]-1,2,4-oxadiazole-HCl, m. 179-80°, 3-[p-chlorobenzyl]-5-piperidinomethyl)-1,2,4-oxadiazole-HCl, m. 157°, 3-[p-chlorobenzyl]-5-[β-pyrrolidinoethyl]-1,2,4-

L4 ANSWER 51 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
oxadiazole-HCl, m. 155°, 3-[β,β-bis(4-chlorophenyl)ethyl]-5-piperidinomethyl-1,2,4-oxadiazole N maleate, m. 117°, 3-[β,β-bis(4-chlorophenyl)ethyl]-5-[β-piperidinoethyl]-1,2,4-oxadiazole N maleate, m. 126°, 3-bis(3,4-dimethoxyphenyl)methyl]-5-[β-piperidinoethyl]-1,2,4-oxadiazole, m. 94° (abs. EtOH), 3-bis(3,4-dimethoxyphenyl)methyl]-5-[β-morpholinoethyl]-1,2,4-oxadiazole, m. 112-15° (abs. EtOH), 3-(α,β-diphenylethyl)-5-[β-piperidinoethyl]-1,2,4-oxadiazole-HCl, m. 196-7° (abs. EtOH), 3-(α,β-diphenylethyl)-5-[β-(N-methylpiperazino)ethyl]-1,2,4-oxadiazole-2HCl, m. 244° (MeOH), 3-[β,β-diphenylethyl)-5-[β-(N-methylpiperazino)ethyl]-1,2,4-oxadiazole, m. 89° (dihydrochloride m. 225-7° (96% EtOH), 3-diphenylmethyl-5-[β-(N-methylpiperazino)ethyl]-1,2,4-oxadiazole, m. 97° (dihydrochloride m. 196° (96% EtOH), 3-(p-chlorobenzyl)-5-[β-(N-methylpiperazino) ethyl]-1,2,4-oxadiazole-2HCl, m. 184.5-8.5° (96% EtOH), 3-[bis(3,4-dimethoxyphenyl)methyl]-5-[β-(N-methylpiperazino) ethyl]-1,2,4-oxadiazole-2HCl, m. 219-21° (96% EtOH), and 3-(3,4-dimethoxybenzyl)-5-[β-(N-methylpiperazino) ethyl]-1,2,4-oxadiazole-2HCl, m. 191-3° (96% EtOH). A mist. of 84 g. I in 1310 ml. CCl4 and 24.53 g. p-chlorovaryyl chloride in 170 ml. CCl4 is kept at room temp. 24 hrs. and filtered, the solid suspended in 1500 ml. H2O, and the mixt. kept 24 hrs. and filtered to give 44.59 g. O-p-chlorobenzyl-β,β-diphenylpropionamidoxime (II), m. 145°. II (12.55 g.) and AcO (6 ml.) heated on a water-bath, treated with H2O and CCl4, and the org. phase washed with Na2CO3 soln. and

concd. gives 9.92 g. 3-[β,β-diphenylethyl)-5-(γ-chloropropyl)-1,2,4-oxadiazole (III) (m.p. not given). A mist. of 9.90 g.

III, 45 ml. PhMe, and 8.90 ml. piperidine is refluxed 11 hrs. and filtered

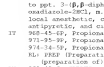
and the filtrate washed with H2O and evapd. to yield 11.20 g. 3-[β,β-diphenylethyl)-5-(γ-piperidinopropyl)-1,2,4-oxadiazole. N maleate m. 166-7° (MeCO2). The γ-morpholinopropyl deriv. is prepd. similarly, N maleate m. 153°. A soln. of 14.53 g. β-chloropropionyl chloride in MeCO was added dropwise with stirring at 0-5° to a suspension of 27.6 g. I and 9.86 g. NaHCO3 in 140 ml. aba. MeCO and the whole stirred 7 hrs. and added to 1380 ml. H2O to yield 27.8 g. O-[β-chloropropionyl]-β,β-diphenylpropionamidoxime (IV), m. 118-17° (abs. EtOH or CHCl3). A soln. of 4.55 g. IV in 25 ml. abs. PhMe and 3 ml. piperidine is refluxed 7 hrs., 20 ml. H2O added, the mixt. evapd. to dryness in vacuo, and the residue treated with HCl in EtOH to gave 2.15 g. 3-[β,β-diphenylethyl)-5-[β-piperidinoethyl)-1,2,4-oxadiazole-HCl, m. 192° (abs. EtOH). O-Chloroacetyl-β,β-diphenylpropionamidoxime, m. 118-19° (obtained similarly to IV), is heated in vacuo at 100-10° 10-15 min. to yield 3-[β,β-diphenylethyl)-5-chloromethyl-1,2,4-oxadiazole, m. 73-4° (MeOH). Heating it with piperidine in PhMe and treating the product with HCl in EtOH yields 3-[β,β-diphenylethyl)-5-[piperidinomethyl)-1,2,4-oxadiazole-HCl,

L4 ANSWER 52 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
m. 187-8° (MeOH). β-Piperidinopropionic acid-HCl (1.97 g.) is added to 2.4 g. 1 in 20 ml. aba. CH2Cl2 at 20°, the mixt. refluxed 2 hrs. and evapd. to dryness in vacuo, the residue in 10 ml. 2N NaOH acid with HCl, the org. phase comcd., and the residue treated with HCl in EtOH

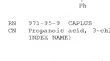
to ppt. 3-[β,β-diphenylethyl)-5-[β-piperidinoethyl)-1,2,4-oxadiazole-2HCl, m. 192-3°. These products showed spasmolytic, local anesthetic, cough-reliever, analgesic, anti-inflammatory, antipyretic, and circulation influencing effects.

IT 968-45-6P, Propionamidoxime, 2,2-diphenyl-, O-chloroacetate
971-95-9P, Propionamidoxime, 2,2-diphenyl-, O-3-chloropropionate
974-34-9P, Propionamidoxime, 2,2-diphenyl-, O-4-chlorobutyrate
RL: PREP (Preparation)
(preparation of)

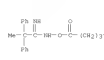
RN 968-45-6 CAPLUS
CN Acetic acid, 5-chloro-, (1-imino-2,2-diphenylpropyl)azanyl ester (CA INDEX NAME)



RN 971-95-9 CAPLUS
CN Propanoic acid, 3-chloro-, (1-imino-2,2-diphenylpropyl)azanyl ester (CA INDEX NAME)

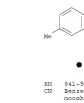


RN 974-34-5 CAPLUS
CN Butanoic acid, 4-chloro-, (1-imino-2,2-diphenylpropyl)azanyl ester (CA INDEX NAME)



L4 ANSWER 53 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:43644 CAPLUS
DOCUMENT NUMBER: 62:43644
ORIGINAL REFERENCE NO.: 62:8374f
TITLE: The resolution of some substituted lactamidines and atrolactamidines by means of the mandelic acids
AUTHOR(S): Ewing, D. F.; Neilson, D. G.
CORPORATE SOURCE: Univ. St. Andrews, Dundee, UK
SOURCE: Journal of the Chemical Society (1965), (Jan.), 770-4
CODEN: JCSOAA; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: English
AB α- and p-Methylatrolactamidines were prepared from the corresponding methylacetophenones and were resolved by means of the mandelic acids. o-Methylacetophenone failed to give an amidine. α-Benzyl-lactamidine was also resolved by means of these acids but β-phenylactamidine showed no separation of the diastereoisomers.
IT 941-52-4 943-23-7 971-52-8
971-53-9
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 941-52-4 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (+)- (9CI) (CA INDEX NAME)

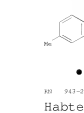
Rotation (+).



● HCl

RN 941-52-4 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (-).

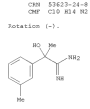


● HCl

RN 943-23-7 CAPLUS

L4 ANSWER 53 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
CN Mandelamidine, α,4-dimethyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

RN 971-52-8 CAPLUS
CN Mandelic acid, (S)-, compd. with (-)-4-hydroxy-m-methylhydratropamidine (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 53623-24-8
CMF C10 H14 N2 O

Rotation (-).

CM 2

CRN 17199-29-0
CMF C8 H8 O3

Absolute stereochemistry. Rotation (+).

RN 971-53-9 CAPLUS
CN Mandelic acid, (R)-, compd. with (+)-p,α-dimethylmandelamidine (1:1)

L4 ANSWER 53 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
(HCl) (CA INDEX NAME)

CM 1

CRN 46347-67-5
CMF C10 H14 N2 O

Rotation (+).

CM 2

CRN 611-71-2
CMF C8 H8 O3

Absolute stereochemistry. Rotation (-).

IT 109535-37-1, Mandelamidine, α-methyl-
(derivs., resolution by mandelic acids)
RN 109535-37-1 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl- (CA INDEX NAME)

IT 941-51-5P, Mandelamidine, p,α-dimethyl-, hydrochloride, isomers 94281-37-5P, Mandelamidine, m,α-dimethyl-, hydrochloride, isomers 95157-76-9P, Mandelic acid, compound with m,α-dimethylmandelamidine (1:1), (+)- 95157-78-1P, Mandelic acid, compound with p,α-dimethylmandelamidine (1:1), isomers RL: PREP (Preparation)
(preparation of)
RN 941-51-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, hydrochloride

L4 ANSWER 53 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
(1:1) (CA INDEX NAME)

● HCl

RN 94281-37-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,3-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 95157-76-9 CAPLUS
CN Benzeneacetic acid, α-hydroxy-, compd. with α-hydroxy-α,3-dimethylbenzeneethanimidamide (1:1) (CA INDEX NAME)

CM 1

CRN 95157-75-8
CMF C10 H14 N2 O

CM 2

L4 ANSWER 53 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

CRN 90-64-2
CMF C8 H8 O3

RN 95157-78-1 CAPLUS
CN Benzeneacetic acid, α-hydroxy-, compd. with α-hydroxy-α,4-dimethylbenzeneethanimidamide (1:1) (CA INDEX NAME)

CM 1

CRN 95157-77-0
CMF C10 H14 N2 O

CM 2

CRN 90-64-2
CMF C8 H8 O3

L4 ANSWER 54 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1965:36363 CAPLUS
DOCUMENT NUMBER: 62:36363
ORIGINAL REFERENCE NO.: 62:6374e-f
TITLE: Electrophilic substitution at saturated carbon. XXIV. Trifluoromethyl as a carbanion-stabilizing group
AUTHOR(S): Cram, Donald J.; Wingrove, Alan S.
SOURCE: Journal of the American Chemical Society (1964), 86(24), 5490-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB *Two systems* have been prepared for study of the stereochem. course of the base-catalyzed H-D exchange at C attached to a trifluoromethyl group. Optically active 2-methyl-3-phenyl-1,1,1-trifluoropropane (I) and the same compound deuterated in the 2-position, and optically active 2-phenyl-1,1,1-trifluorobutane (II) and its deuterated counterpart (2-position) were examined. In tert-BuOD at 124°, (+)-I was found to undergo elimination reaction to the exclusion of isotopic exchange. The initially formed 1,1-difluoro-2-methyl-3-phenyl-1-propene underwent a base-catalyzed allylic rearrangement to give a 6.5:1 mixture of trans- to cis-3,3-difluoro-2-methyl-1-phenyl-1-propene (trans- to cis-III), which were identified by their spectral properties. The base-catalyzed elimination reaction exhibited a kinetic isotope effect of 1.2, a fact which suggests a carbanion intermediate for the reaction. II also underwent elimination to give 1,1-difluoro-2-phenyl-1-butene and its polymers. However, H-D exchange also occurred, but at a much slower rate. In tert-BuOH-tert-BuOK, and in EtOH-KOEt, isotopic exchange went with total racemization (km/ks, the ratio of the rate constant for exchange to the rate constant for racemization, was equal to unity). In MeOH-KOMe, or MeOH-MeOLi, isotopic exchange went with net inversion (km/ks, ranged from 0.60 to 0.84, depending on whether the substrate or the solvent was D labeled). This result is interpreted in terms of an aggs.-solvated syn. and dissociated carbanion.
IT 941-50-4 941-51-5 941-52-6 943-23-7 971-52-4 971-53-5 94281-37-5 95157-76-9
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 941-50-4 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

● HCl

L4 ANSWER 54 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

RN 941-51-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 941-52-6 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

● HCl

RN 943-23-7 CAPLUS
CN Mandelamidine, n,α-dimethyl-, monohydrochloride, (-)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 54 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
(8CI) (CA INDEX NAME)

CM 1

CRN 46347-67-5
CMF C10 H14 N2 O

Rotation (+).

CM 2

CRN 611-71-2
CMF C8 H8 O3

Absolute stereochemistry. Rotation (-).

RN 94281-37-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,3-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 95157-78-1 CAPLUS
CN Benzeneacetic acid, α-hydroxy-, compd. with α-hydroxy-α,4-dimethylbenzeneethanimidamide (1:1) (CA INDEX NAME)

CM 1

CRN 95157-77-0
CMF C10 H14 N2 O

L4 ANSWER 54 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

● HCl

RN 971-52-8 CAPLUS
CN Mandelic acid, (R)-, compd. with (-)-α-hydroxy-n-methylhydratropamidine (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 53623-24-9
CMF C10 H14 N2 O

Rotation (-).

CM 2

CRN 17199-29-0
CMF C8 H8 O3

Absolute stereochemistry. Rotation (+).

RN 971-53-9 CAPLUS
CN Mandelic acid, (R)-, compd. with (+)-β,α-dimethylmandelamidine (1:1)

L4 ANSWER 54 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

CM 2

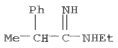
CRN 90-64-2
CMF C8 H8 O3

L4 ANSWER 55 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1962:435850 CAPLUS
DOCUMENT NUMBER: 57:35850
ORIGINAL REFERENCE NO.: 57:7081i,7082a-d
TITLE: The structure of N-mono- and N,N'-disubstituted amidines
AUTHOR(S): Prevorsek, Dusan C.
CORPORATE SOURCE: Textile Res. Inst., Princeton, NJ
SOURCE: Journal of Physical Chemistry (1962), 66, 769-78
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

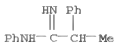
AB Factors influencing the position of tautomeric equilibrium of a number of N-mono- and N,N'-disubstituted amidines were studied by infrared spectral analyses. In solution the unsubstituted amidines, RC(:NR')NH2 .dblarw. RC(:NH)NHR' (I) (R' = H), existed as a mixture of approx. equal amts. of each tautomer. The equilibrium of I was found to be displaced in proportion to the electroneg. of the substituents R'. Thus, when R' was phenyl or hydroxyl (amidoximes), the equilibrium was shifted to a the left, whereas an ethyl group shifted the equilibrium to the right. The nature of the R group apparently was without effect. Characteristic frequency assignments in the 2-7° region for eight N-monosubstituted amidines and seven amidoximes were given where R varied from 2-thienyl, 2-, 3-, or 4-piperidyl, benzyl, α-phenethyl, α-phenylpropyl, and αphenylbutyl groups, R' = H, and R'' = hydroxyl, phenyl, methyl, or ethyl. The spectra of N,N'-disubstituted amidines (II) in dilute solution showed two bands in the 3 μ region, b suggesting the presence of either two forms of a monomer or a single form giving rise to both bands. Geometric isomerism with respect to the C:N bond was felt unlikely because of the steric effects offered by the R' and R'' groups (substituted phenyl or naphthyl groups). The possibility that one band was an overtone of the fundamental C:N stretching vibration in the 6 μ region was also deemed improbable. Simple tautomerism could not explain the two bands, since identical configurations would result when R' = R''. It was concluded, however, that N,N'-disubstituted amidines very probably exhibited in solution tautomerism leading to a rotational isomerism with respect to both single and double CN bonds. This would explain the appearance of two N-N and C:N bands for derivs. with identical substituents. Characteristic frequency assignments in the 2-7 μ region for ten N,N'disubstituted amidines were given where R = methyl, α-phenethyl, and α-phenylpropyl, R' and (or) R'' = ethyl, phenyl, substituted phenyl, or β-naphthyl. The infrared spectra of these N-mono- and N,N'-disubstituted amidines d indicated an electronic configuration similar to that of amides. All the amidines studied were prepared according to known procedures.

IT 91429-53-7P, Hydratropamidine, N-ethyl- 92579-12-9P, Hydratropamidine, N-phenyl-

L4 ANSWER 55 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
RL: PREP (Preparation)
(prepn. of)
RN 91429-53-7 CAPLUS
CN Benzeneethanimidamide, N-ethyl-α-methyl- (CA INDEX NAME)



RN 92579-12-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-N-phenyl- (CA INDEX NAME)

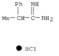


L4 ANSWER 56 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1962:410679 CAPLUS
DOCUMENT NUMBER: 57:10679
ORIGINAL REFERENCE NO.: 57:2141d-i,2142a-b
TITLE: Amidines and other derivs. of phenylalkylacetic acids
AUTHOR(S): Delaby, Raymond; Reynaud, Pierre; Lilly, Franck
SOURCE: Bulletin de la Societe Chimique de France (1961) 2067
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:10679

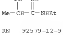
AB Starting with phenylalkylacetonitriles, the title compds. were prepared in order to ascertain their possible hypocholesterolemic action (Redel and Cottet, CA 48, 13061i; C., et al., 13975c). The first step was the preparation of the HCl salt of the imino ester; e.g., PhMeCHC(:NH)OEt.HCl (I) was prepared by passing a current of HCl into a mixture of 20 g. PhMeCHCN (II), 40 cc. Et2O, and 40 cc. absolute EtOH at 0-5° 2.5 hrs. and keeping 2 days at 0°. After removing the solvent in vacuo the residual oil was crystallized from Et2O to yield 92% I, m. 106°; free imino ester (III) b13 116°, n23D 1.5064. PhMeCHC(:NH)NH2.HCl (IV) resulted when 10 g. I in 40 cc. EtOH was treated with NH3 0.5 hr., then refluxed 0.5 hr., the solvent distilled in vacuo, and the residue crystallized from hot H2O; yield, 8.5 g. IV, m. 235°. The following PhCHRC(:NH)OEt.HCl were obtained (R, % yield, m.p., b.p., b.p. pressure (mm.) given): Me, 92,106°,-,-; Et, 87, 98°, -, -; Pr, 83, 82°, -, -. The data for PhCHRC(:NH)OEt were: Me, 82, -, 116°, 13; Et, 84, -, 121°, 15; Pr, 81, -, 103°, 1. The data for PhCHRC(:NH)NH2,HCl were: Me, 98, 235°, -, -; Et, 99, 232°, -, -; Pr, 99, 238°, -,-. Mono- and dialkylamidines were obtained by the action of AlCl3 (V) on a mixture of nitrile and amine. The following PhCHRC(:NH)NR'R''.HCl were prepared (R, R', R'', % yield, b.p./mm., and m.p. given): H, H, Et, 85, 110°/0.1, 61°; H, Et, Et, 68, 131°/2.5, -; H, H, Ph, 95, -, 138°; Me, H, Et, 75, 109°/0.2, -; Me, Et, Et, 62, 111°/0.1, -; Me, H, Ph, 84, -, 89°; Et, H, Et, 99, 115°/0.15, -; Et, Et, Et, 50, -, 45°; Et, H, Ph, 91, -, 86°; Pr, H, Et, 67, 152°/3, -; Pr, Et, Et, 54, 102°/ 0.01, -; Pr, H, Ph, 96, -, 110.5°; n-C8H17, H, Et, 75, 143°/0.1, -; n-C8H17, Et, Et, 53, 160°/0.3, -; n-C8H17, H, Ph, 62, -, 52°. The acids were prepared by saponification of the nitriles. E.g., a solution of 86 g. KOH and 50.3 g. II in 400 cc. EtOH was refluxed 16 hrs. (NH3 evolution was virtually complete in 12 hrs.), the EtOH distilled in vacuo, the residue dissolved in H2O and extracted with Et2O to remove neutral compds. (less than 0.2 g.), the H2O layer acidified, and the free acid extracted from it with Et2O; yield, 89% PhMe-CHCO2H (VI), b13 145°, m. about 16%, n24D 1.5210. VI was converted by SOCl2 into 96% PhMeCHCOCl (VII), b13 100-1°. The following PhCHRCO2H and chlorides were prepared (R, m.p., b.p./mm., and % yield of acid, and b.p./mm. and % yield of chloride given): H, 78°, 144°/12, 92, 95°/14, 88; Me, about 16°,

L4 ANSWER 56 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
145°/13, 89, 101°/13, 96; Et, 42°, 158°/15, 85, 112°/16, 97; Pr, 52% 167°/15, 90, 118°/13, 96; n-C8H17, -, 170-3°/0.3, 93, 138°/0.3, 88. The various amides were prepd. from the COCl derivs.; e.g., 8.5 g. VII and 5 g. EtNH2 were each dissolved in 75 cc. C6H6, stirred together, and refluxed 0.5 hr. (1 hr. for the higher homologs). After cooling, EtNH2.HCl was dissolved in H2O, the soln. extd. with Et2O and the ext. added to the C6H5 layer, dried over Na2SO4, and the solvents removed in vacuo. The residue of PhMeCHCONHEt crystd. on cooling; yield after 2 crystns. from C6H6-petr. ether (8:92) 83%, m. 65.5-6°. PhMeCHCONH2 was prepd. similarly, using excess NH3 and not allowing the temp. to exceed 65°; yield 83% after crystn. from C6H6, m. 92.5°. The following PhCHRCONR'R'' were prepd. (R, R', R'' 157°;, H, H, Et, 96, -, 69, 5°; H, Et, Et, 98, 119°/0.3, -; H, H, Ph, 95, -, 113°; H, H, PhCH2, 93, -, 119°; Me, H, H, 89, -, 92.5°; Me, H, Et, 95, -, 66°; Me, Et, Et, 94, 105°/0.15, about 16°; Me, H, Ph, 94, -, 134°; Me, H, PhCH2, 96, -, 75°; Et, H, H, 97, -, 84°; Et, H, Et, 93, -, 66°; Et, Et, 96, 115°/0.2, 32°, 5; Et, H, Ph, 98, -, 97°; Et, H, PhCH2, 93, -, 82°; n-C8H17, H, H, 99, -, 86°; n-C8H17 H, Et, 95, -, 53°; n-C8H17 Et, Et, 98, 168-9°/0.2, -; n-C8H17 H, Ph, 93, -, 66°; n-C8H17 H, PhCH2, 99, -, 52°.

IT 78622-24-9P, Hydratropamidine, hydrochloride 91429-53-7P, Hydratropamidine, N-ethyl- 92579-12-9P, Hydratropamidine, N-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 78622-24-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



RN 91429-53-7 CAPLUS
CN Benzeneethanimidamide, N-ethyl-α-methyl- (CA INDEX NAME)



RN 92579-12-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-N-phenyl- (CA INDEX NAME)

L4 ANSWER 56 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

L4 ANSWER 57 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1962:400752 CAPLUS
DOCUMENT NUMBER: 57:752
ORIGINAL REFERENCE NO.: 57:128b-c
TITLE: Complexes formed by a-hydroxy amidines with transition metal ions. I. Acid dissociation constants of ligands
AUTHOR(S): Gould, E. C.; Jameson, R. F.
CORPORATE SOURCE: Queen's Coll., Dundee, GB
SOURCE: Journal of the Chemical Society (1962) 29C-9
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The first-order rate constants for the decomposition of (S)-HOC(Ph)(R)C(:NH)NHR [R = H (I); R = Me (II); and R = Et (III)] at 250 are 18.0 (I), 8.4 (II), and 8.3 (III) + 1-5/sec., the acid dissociation constants, pK and pK2, at 25° are I, 10.82 ± 0.01 and 12.52 ± 0.05; II, 10.96 ± 0.01 and 12.72 ± 0.05; and III, 11.06 ± 0.01 and 12.86 ± 0.05.
IT 92442-87-9, Mandelamidine, a-methyl-, hydrochloride (decomposition and ionization of)
RN 92442-87-9 CAPLUS
CN Benzeneethanimidamide, a-hydroxy-a-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● xHCl

L4 ANSWER 58 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1961:47579 CAPLUS
DOCUMENT NUMBER: 55:47579
ORIGINAL REFERENCE NO.: 55:9145i,9141a
TITLE: Complexes formed by a-hydroxy amidines with transition metal ions
AUTHOR(S): Gould, E. C.; Jameson, R. F.; Neilson, D. G.
CORPORATE SOURCE: Queen's Coll., Dundee, UK
SOURCE: Proceedings of the Chemical Society, London (1960) 314-15
CODEN: PCSLAW; ISSN: 0369-8718
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Reaction of moist Ag2O with PhMeCOCl(:NHCl)NH2 gave an atrolactanidine which could not be freed from Ag. Reaction of a-hydroxy amidines PhRC(OH)C(:NH)NHR2 [R = H, Me, or Et) with Cu++ or Ni++ gave colored complexes. Bis[mandelamidine]nickel(II), obtained by extraction from aqueous solution with AmOH, was pink and diamagnetic, suggesting the square planar configuration, but the characteristic absorption at 25,000 cm.-1 was absent. Assuming octahedral coordination, if the band at 20,200 cm.-1 was assigned to the 3T1g(F) transition, the 3T2g and 3T1g(P) bands should have been at 13,500 and 34,000 cm.-1 Such bands were observed at 16,000 and 34,000 cm.-1, suggesting octahedral configuration, possibly involving solvent mols. Titration data indicated the mandelamidinium ion is a dibasic acid, pK1 10.5, pK2 12.2.
IT 109595-37-1P, Atrolactanidine, complex with Ni
RL: PREP (Preparation)
(formation of)
RN 109595-37-1 CAPLUS
CN Benzeneethanimidamide, a-hydroxy-a-methyl- (CA INDEX NAME)

L4 ANSWER 59 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1959:82995 CAPLUS
DOCUMENT NUMBER: 53:82995
ORIGINAL REFERENCE NO.: 53:14925i,14930a-e
TITLE: Stereochemical structure. XII. Resolution of (±)-atrolactanidinium chloride
AUTHOR(S): Kopys, R.; Neilson, D. G.
CORPORATE SOURCE: Queen's Coll., Dundee, UK
SOURCE: Journal of the Chemical Society (1959) 688-90
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 49, 13255e. (±)-Atrolactanidinium chloride (I) was prepared from PhAc cyanohydrin (II) via Et (±)-atrolactimidate·HCl (III). (±)-Atrolactanidine (IV) was resolved by separation of the diastereoisomeric salts with optically active mandelic acid (V). (-)-Atrolactic acid (VI), isolated from (-)-atrolactanidinium chloride (VII), was of at least 90% optical purity. PhAc (120 g.) in 90 ml. EtOH and 123 g. NaCN in 150 ml. H2O treated at 5° during 2 hrs. with 210 ml. concentrated HCl, the EtOH layer separated and the aqueous layer again extracted with EtOH, and the ethereal exts. distilled gave 48 g. II, b18 147-9°, yellow oil. II (48 g.) and 16 g. anhydrous alc. treated 48 hrs. at 0° with 13.2 g. dry HCl and EtOH gave 60 g. III, m. 101-2° (decomposition). III (5 g.) treated with 12 ml. 40 NaOH gave 2 g. Et (±)-atrolactimidate, m. 56-7° (ligroine). An anhydrous solution of 8.5 g. NH3 in 100 ml. alc. shaken 12 hrs. with 23 g. III and the solution evaporated at room temperature gave 17 g. I, m. 174-5° (dilute HCl). I (6 g.) shaken at 0° with 15 ml. 12N NaOH and H2O added gave 3.7 g. IV, m. 77-8° (decomposition); picrate m. 188-9°. I (2.5 g.) heated with 2.2 g. Na salt V in H2O to a clear solution gave 1 g. (±)-atrolactanidine (+)-mandelate (VIII), m. 155-6° (H2O). I (6.7 g.) and 5.8 g. Na (+)-mandelate heated in 37 ml. H2O gave 2 g. (-)-atrolactanidine (+)-mandelate (IX), m. 165° (decomposition), [α]18546l 12.1° (c 0.91, MeOH). Ethereal (+)-mandelic acid (1.5 g., [α]5461 186° (MeOH)), mixed with 1.4 g. IV in alc. gave 0.7 g. IX. (+)-Atrolactanidine (-)-mandelate (X) was prepared as in the above method but with (-)-mandelic acid. X softened at 162°, m. 165° (decomposition), [α]16546l -12.5° (c 0.86, MeOH). IX set aside 24 hrs. with excess HCl-Et2O gave VII, m. 200-1° (decomposition), [α]15546l -55.6° (c 0.54, H2O). Similarly X yielded (-)-atrolactanidinium chloride, softened at 197°, m. 201° (decomposition), [α]15546l (c 0.58, H2O); the yield was almost theoretical. VII (0.5 g.) heated in 4N NaOH until evolution of NH3 ceased, the solution acidified, and extracted with Et2O gave 0.2 g. V), [α]22D -48.3° (c 0.55, H2O). The 2 forms of I treated at 0° with alkaline sols. of varying strengths did not give crystalline products. The rotatory powers of the optically active forms of I at 3 wavelengths in the visible spectrum gave approx. straight line Lowry-Dickson plots but the detns. were not sufficient to warrant discussion.
IT 92442-87-9 109595-38-2
(Derived from data in the 4th Collective Formula Index (1957-1961))

L4 ANSWER 59 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 109595-38-2 CAPLUS
CN Benzeneacetic acid, α-hydroxy-, compd. with α-hydroxy-α-methylbenzeneethanimidamide (1:1) (CA INDEX NAME)

CM 1

CRN 109595-37-1
CMF C9 H12 N2 O

CM 2

CRN 90-64-2
CMF C8 H8 O3

IT 1071532-18-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(therochemical structure, X11. Resolution of (2)-atrolactamidinium chloride)
RN 1071532-18-7 CAPLUS
CN Benzeneethanimidamide, α-methyl-α-(2,4,6-trinitrophenoxy)-

L4 ANSWER 60 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1959:82994 CAPLUS
DOCUMENT NUMBER: 53:82994
ORIGINAL REFERENCE NO.: 53:14929i
TITLE: Thermal oxidation of methyl esters of fatty acids
AUTHOR(S): Ramanathan, Venkatachalan
CORPORATE SOURCE: Univ. of Illinois, Urbana
SOURCE: (1959) 95 pp. Avail.: Univ. Microfilms (Ann Arbor, Mich.), Order No. 59-564
From: Dissertation Abstr. 19, 2907-8
DOCUMENT TYPE: Dissertation
LANGUAGE: Unavailable
AB Unavailable
IT 92442-87-0 109595-38-2
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 109595-38-2 CAPLUS
CN Benzeneacetic acid, α-hydroxy-, compd. with α-hydroxy-α-methylbenzeneethanimidamide (1:1) (CA INDEX NAME)

CM 1

CRN 109595-37-1
CMF C9 H12 N2 O

CM 2

CRN 90-64-2
CMF C8 H8 O3

L4 ANSWER 59 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

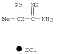
IT 109595-37-1, Atrolactamidine, (-)-
(and derivs.)
RN 109595-37-1 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl- (CA INDEX NAME)

L4 ANSWER 60 OF 62 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

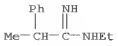
ACCESSION NUMBER: 1958:113428 CAPLUS
DOCUMENT NUMBER: 52:113428
ORIGINAL REFERENCE NO.: 52:20024g-i,20025a
TITLE: Research on hypocholesterol. Synthesis of amidines from substituted phenylacetic acids
AUTHOR(S): Delaby, Raymond; Reynaud, Pierre; Lilly, Frank
SOURCE: Compt. rend. (1958), 246, 2905-6
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB PhCH2CN with Et2CO3 in the presence of EtONa gives Et α-cyanophenylacetate, converted by treatment with alkyl halides (RX) and saponification with NaOH to PhCHRCN, e.g. 62% PhCHMeCN, b15 108°, 69% PhCHEtCN, b15 115° 72% PhCHPrCN, b14 130°, and 63% PhCH(C8H17-n)CN, b0.1 133°. On passing dry HCl into solns. of the nitriles in EtOH, the iminoesters are formed, and addition of amines in the presence of AlCl3 gives N-substituted amidines. Thus, PhCHMeCN with HCl and EtOH gives PhCHMeC(:NH)OEt.HCl, m. 103.5°, and then PhCHMeC(:NH)NH2.HCl, m. 235°, is ethylated to PhCHMeC(:NH)NHEt, b0.2 109°, and PhCHMeC(:NH)NEt2, b0.1 111°, or phenylated to PhCHMeC(:NH)NHPh, m. 89°. Similarly, PhCHEtCN gives PhCHEtC(:NH)OEt.HCl, m. 98° then PhCHEtC(:NH)NH2.HCl, 232°, PhCHEtC(:NH)NHEt, b0.15 115°, or PhCHEtC(:NH)NEt2, m. 45°, and PhCHEtC(:NH)NHPh, m. 86°. Also, PhCHPrCN gives PhCHPrC(:NH)OEt.HCl, m. 82°, then PhCHPrC(:NH)NH2.HCl, m. 238°, PhCHPrC(:NH)NHEt, b3 152°, or PhCHPrC(:NH)NEt2, b0.1 102° and PhCHPrC(:NH)NHPh, m. 110.5°. PhCH(C8H17-n)CN gives the amidines PhCH(C8H17-n)C(:NH)NEt2, b0.3 160°, and PhCH(C8H17-n)-C(:NH)NHPh, m. 52°. The physiol. activity of the substituted amidines is being studied.

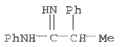
IT 78622-24-9P, Hydratropamidine, hydrochloride 91429-53-7P, Hydratropamidine, N-ethyl- 92579-12-9P, Hydratropamidine, N-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 78622-24-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



RN 91429-53-7 CAPLUS
CN Benzeneethanimidamide, N-ethyl-α-methyl- (CA INDEX NAME)



RN 92579-12-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-N-phenyl- (CA INDEX NAME)



ACCESSION NUMBER: 1949:38809 CAPLUS
DOCUMENT NUMBER: 43:38809
ORIGINAL REFERENCE NO.: 43:6993c-i,6994a-b
TITLE: Aliphatic nitro compounds. XIX. Friedel-Crafts reactions with α- and β-nitro olefins
AUTHOR(S): Lambert, A.; Rose, J. D.; Weedon, B. C. L.
SOURCE: Journal of the Chemical Society (1949) 42-6
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 42, 4917e. CH2:CMeCH2NO2 (I) (10 g.), added (15 min.) to 16 g. AlCl3 in 50 cc. C6H6 at 30°, stirred 1 hr. at 30-40°, and poured onto concentrated HCl and ice, gives 9.55 g. 1-nitro-2-phenyl-2-methylpropane (II), b0.1 67-70°, nD23 1.5235; II results in 13-g. yield from PhMgBr (9.6 g. Mg) in 300 cc. ether on addition (1.5 hrs.) to 40 g. Me2C:CHNO2 in 300 cc. H2O at -5 to 0°, refluxing 0.5 hr., and decomposing with 24 g. AcOH in 160 cc. H2O. Reduction of 4 g. II in 50 cc. MeOH over Raney Ni at room temperature and atmospheric pressure gives 2.5 g. 2-phenyl-2-methylpropylamine, b14 96-8° (picrate, yellow, m. 160°). I (10 g.) in 100 cc. PhMe, saturated with BF3, kept at room temperature overnight, and heated 1 hr. at 70-80°, gives 5 g. 1-nitro-2-p-tolyl-2-methylpropane (III), pale yellow, b0.5 85-90°, b13 145-50°, nD22 1.5258. III (0.4 g.), boiled 4 hrs. with 3 g. KMnO4 in 25 cc. H2O, gives 0.3 g. α,α-dimethylhomoterephthatic acid (IV), m. 236-7°. Catalytic reduction (as above) of 3.6 g. III yields 2.5 g. 2-p-tolyl-2-methylpropylamine, b10 111.5-15°, b32 134°, nD22 1.5231 (picrate, yellow, m. 211-13°). Me2C:CHNO2 (20 g.) in 100 cc. PhMe, saturated with BF3 at 50°, gives 8.5 g. α-(p-tolyl)isobutyrohydroxamic acid (V), m. 157°, gives a deep red-violet color with FeCl3, and reduces AgNO3 in NH4OH. Distillation of the residue from the PhMe yields 6 g. III and a small quantity of a compound (C11H13ON ?), m. 132-4°. Catalytic reduction of 0.9 g. V in MeOH yields 0.5 g. α-(p-tolyl)isobutyramide (VI), m. 143-4°. VI (0.2 g.) and 15 cc. 2 N HCl, refluxed 10 hrs., give 0.17 g. α-(p-tolyl)isobutyric acid (VII), m. 82°; VII results also on refluxing 0.5 g. V and 15 cc. 2 N HCl 0.5 hr. The structures of the VII reported by Wallach [Nachr. Ges. Wiss. Gottingen 2, 4(1899)] and by Rupe and Burgin (C.A. 5, 2841) are not clear. The Na derivative from 98 g. p-MeC6H4CH2CN (prepared with NaNH2), treated dropwise with 213 g. MeI (1 hr.), gives 42% α-(p-tolyl)isobutyronitrile, b12 122-3°, b763 246°, nD22 1.5106, d2222 0.9661; hydrolysis with KOH yields VI and VII. Oxidation of 4 g. VII in 40 cc. 5% Na2CO3 with 240 cc. 4% KMnO4 (1 hr.) gives 4 g. IV; further oxidation gives p-C6H4(CO2H)2. Details are given of the attempted preparation of VII by the method of R. and B. Me2C:CHNO2 and C6H6 do not yield a hydroxamic acid with BF3. Me2C:CHNO2 (60 g.), added (1 hr.) to 80 g. AlCl3 in 300 cc. C6H6 at 40°, the mixture stirred an addnl. hr., decomposed with HCl and ice, and extracted with C6H6, gives 25 g. α,β-dichloroisobutyraldoxime, Me2CClCCl:NOH, b14 81-5°, nD25 1.4922, and 22 g. α-phenylisobutyrohydroxamyl chloride (VIII), Me2PhCCCl:NOH, m. 73-4°. VIII and PhNH2 in EtOH give α-phenylisobutyrohydroxamanilide, m. 171-2°. VIII (5 g.) and 2.1 g. NaHCO3 in 100 cc. H2O, shaken 0.5 hr., give 2 g.

1-phenylisopropyl isocyanate (IX), b0.16 50-2°, nD22 1.5038; with PhNH2 it yields 1-phenyl-3-(1-phenylisopropyl)urea, m. 193-4°. IX (0.6 g.), refluxed 3 hrs. with aq. NaHCO3, gives 0.4 g. 1,3-bis(1-phenylisopropyl)urea, (PhMe2CNH)2CO, m. 226-7°. Hydrogenation of 4 g. of IX over Raney Ni gives 1.6 g. 1-methyl-1,3-bis(1-phenylisopropyl)urea, PhMe2CNMeCONHC-PhMe2, m. 171-2°. MeCH(OH)CHNO2 (50 g.), C6H6, and AlCl3, refluxed 4 hrs., give 23% PhCH:NOH and 9 g. MeCHPh2; this can be explained by the initial formation of MeNO2 and MeCHO. MeNO2 and C6H6 give PhCH:NOH and PhN:CHPh.

IT 858208-39-6P, Hydratropanilide, α-methyl-, oxime
RL: PREP (Preparation)
(preparation of)
RN 858208-39-6 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α,α-dimethyl-N'-phenyl- (CA INDEX NAME)